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Exciton bleaching and electron teleportation driven by magnetic field in dilute GaAs(N) quantum wells

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The Hamiltonian for two harmonic oscillators in the basic of angular momentum \( j = 1/2 \) and magnetic quantum numbers \( m_j = 1/2, -1/2 \) is build. Proportion coefficient are expressed by means of Clebsh-Gordan coefficient. It is shown that formalism may be applicable at the explaining of deformation dependence of the fundamental band gap of dilute GaInNAs. It is shown that formalism allows to predict the magnetic Coulomb levels near anticrossing point which are created at the generation two conduction band (\( \Delta_{c1} \) and \( \Delta_{c2} \)) in GaN/AlN quantum wells. The two solutions in the dispersion equation which lead to a duality of conduction band with highly nonparabolic stage are found. The additional optical transitions are found. The bound states at the research of transitions of discrete spectrum into the continuous state are found. The analytical expression of Landau quantization in dilute GaAsN and their wave vectors are found. It is shown that the consideration of dilute GaAsN is united with the research of 1D periodical crystal in the direction of perpendicular to the magnetic field. In the article the conduction bands of dilute GaAsN, in the case when \( n^{(2)} \to \infty \) are studied. For 0.1% N with 0.2 eV localized N-impurity level with respect of edge conduction band and hybridization between extended states of semiconductor matrix and orbits of N atoms occurs at \( k = 6 \times 10^6 \text{m}^{-1} \) calculated from Brillouin zone center, need to apply of magnetic field of 15.4 T, in order to tune an electron into a given \( k \) state. Thus it is shown, that the formalism can be used in the magnetotunneling spectroscopy researches. In this paper, we present microscopic calculations of the absorption spectra for GaN/AlGaAs \( \to \) N quantum well systems. Whereas quantum well structures with parabolic law of dispersion exhibit the usual bleaching of the exciton resonance without shifting spectral position, a significant red-shift of the exciton peak is found with increasing electron-hole gas density for wurtzite quantum well. Electron and photon teleportation in quantum spectroscopy researches associates with a significant red-shift of the exciton peak in materials with complex dispersion. The energy of the exciton resonance for the wurtzite quantum well is found. The obtained results can be explained by an influence of the valence band structure on quantum confined effects. The optical gain spectrum in Hartree-Fock approximation is calculated. Sommerfeld enhancement is calculated. The red shift of the gain spectra in Hartree-Fock approximation with respect to Hartree gain spectra is calculated. The entanglements of doubled conduction band one can lead into electron teleportation, quantum cryptography and artificial intelligence researches.

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I. INTRODUCTION

Dilute nitrides have recently attracted considerable attention due to found new electrical and optical properties. It has been found that the substitution of the V anions in III-V compound with small amounts of nitrogen causes the drastic changes of the electronic properties. These enclose a reduction of the fundamental band-gap energy, a significant increase in electron effective mass and a decrease in electron mobility. \(^1\)\(^-\)\(^3\). A new optical transition above the fundamental band-gap energy has been observed.\(^1\)\(^,\)\(^2\). The strong effect of N on the band gap is related to the fact that replacement of atoms As with the much smaller and more electronegative N atom leads to a large, local perturbation of the crystal lattice potential.

Since the effect of nitrogen on the electronic band structure and optical properties of dilute nitrides can be consistently described in terms of an anticrossing interaction between localized nitrogen states of the semiconductor matrix, it is interesting to consider envelope wave vector formalism for GaAsN. In a simplest approach based on the virtual crystal approximation.

The highly localized nature of the N states suggest that there is weak hybridization between the orbits of N atoms and the extended states of semiconductor matrix.

It is assumed that the spatial distribution of the impurity atoms is random and homogeneous. The application of this model is in principle limited to dilute impurity concentration for which the distance between neighbouring impurity atoms is much larger than the spatial extension of wavefunction of the N resonant states.\(^1\)\(^,\)\(^5\).

In the paper \(^2\) the deformation dependence of the fundamental band gap of a few Ga\(_{1-x}\)In\(_x\)N\(_y\)As\(_{1-y}\) samples were
researched by photomodulated transmission measurements. For the case without N contents in Ga$_{1-x}$In$_x$N$_y$As$_{1-y}$, the band gap increases linearly with applied hydrostatic pressure. With N contents a much weaker dependence of the band gap energy at low pressures and a tendency of energy gap to saturate at high pressures are observed. This type of behavior is observed for group III-V semiconductors. Adding N changes the pressure dependence. The saturation is clearly visible with lower N contents. In this studies need to consider uniting there effects: anticrossing

This type of behavior is observed for group III-V semiconductors. Adding N changes the pressure dependence. The band gap increases linearly with applied hydrostatic pressure. With N contents a much weaker dependence of the band gap. Here obviously a pressure-induced crossover of noninteracting Γ and X conduction band valleys and hydrostatic pressure from which is depended fundamental band gap. The linear nature of the transformation suggests that it cannot associated with a pressure-induced crossover of noninteracting Γ and X conduction band valley. It rather indicates about two strongly interacting energy levels with distinctly difference deformation or magnetic dependence in connection with existing the analogy between the deformations and magnetic field applied along [111]. The pronounced change in the deformation dependence of the energy gap can be understood in terms of a pressure-induced transformation of the nature of the lowest conduction band states, which change from extended to highly localized.

The intrinsic wurtzite effect, band folding has been observed in III nitrides. The created band folding effect suggests that the structure of III nitrides is transformed from cubic zinc-blende to hexagonal wurtzite. Two conduction band (Δ$_{c1}$ and Δ$_{c3}$) are generated when direction of the wave vector along Γ-L [111] of zinc-blende is folded back to Γ-A [0001] direction of wurtzite.

A few tops in energy spectrum of GaN quantum well under tensile biaxial strain are found. As the tensile biaxial strain grows, the remote from Brillouin zone center top shifts up with respect Γ point.

For two conduction bands a band crossing occurs along Γ-A direction. The crossing point is a mathematical saddle point. A few tops in energy spectrum of GaN quantum well under tensile biaxial strain are found. As the tensile biaxial strain grows, the remote from Brillouin zone center top shifts up with respect Γ point.

Near Γ-point Δ$_{c1}$ band is an s-like state, while Δ$_{c3}$ band is a highly hybrid sp$^3$ state. It has much higher p wave probability at the calculations spin dependence of full band structure in the method of linear combination of atomic orbitals. Since Γ$_{c3}$ point is indeed folded back from L$_{c1}$ point of zinc-blende.

A different mechanism (Δ$_{c1}$-Δ$_{c3}$) coupling accounts for the spin splitting of wurtzite GaN, that originated from the intrinsic wurtzite effects (band folding and structure inversion asymmetry). The band-folding effect generates two conduction bands (Δ$_{c1}$ and Δ$_{c3}$), in which p-wave probability has tremendous change when $k_z$ approaches the anticrossing zone. The spin-splitting energy induced by Δ$_{c1}$-Δ$_{c3}$ interaction and wurtzite structure inversion asymmetry are much larger than traditional Rashba and Dresselhaus effects. Tsubaki et al. and Lo et al. were observed a large spin-splitting energy (greater than 5 meV). When to apply the voltage to GaN/AlN quantum well, can found that the spin-splitting energy is sensitively controllable by an electric field. Based on the mechanism, a p-wave enhanced spin-polarized field effect transistor, made of In$_x$Ga$_{1-x}$N/In$_y$Ga$_{1-y}$N for spintronics application were proposed by authors.

The entanglements of doubled conduction band one can lead into electron teleportation, quantum cryptography and artificial intelligence researches.

A. Electron and photon teleportation in quantum spectroscopy researches of exciton bleaching in materials with complex dispersion

The physical properties of wide bandgap group-III quantum well systems are under investigation due to their application in light emitters and semiconductor lasers in the ultraviolet, blue and green wavelength region. Ultraviolet light-emitting diodes and lasers have recently obtained considerations due to applications in compact biological detection systems, analytical devices and medical diagnostics. A number of light-emitting diodes and laser diodes have been demonstrated. However these structures are in the developmental stage and there are many questions with respect performance and device configurations.

Realizing the deep-ultraviolet semiconductor-based light-emitting diodes provides light sources for various applications, for instance to the biological detection and data storage. Although such devices principally need Al$_y$Ga$_{1-y}$N - based quantum well with a high Al contents, their fundamental optical properties remain discussion. It has been proved experimentally that surface emission from [0001] - oriented Al$_y$Ga$_{1-y}$N is quite weak because of the predominant optical polarization along the [0001] c direction. The explanation of these effects may be found from the structure of valence band in AlN different from that in GaN. In wurtzite GaN or AlN the degeneracy of the p-like states at the Γ point is lifted by both crystal-field splitting and spin-orbit splitting leading to forming three valence bands at the Brillouin zone center.

Since AlN has a negative crystal field splitting energy while GaN has a positive, than these splitting lead to arrangements of valence bands in AlN in the order of Γ$_7$, Γ$_9$ and Γ$_7$, while GaN Γ$_9$, Γ$_7$ and Γ$_7$. Because the
Figure 1. (Color online) Calculated Hartree-Fock absorption spectra for the quantum well of width of 2.6 nm at concentration of carriers $n = p = 5 \times 10^{11}$ cm$^{-2}$ (Curve 1), $n = p = 10^{11}$ cm$^{-2}$ (Curve 2), $n = p = 0$ cm$^{-2}$ (Curve 3) at temperature 300 K.

topmost of valence band in AlN has the crystal field split off holes with $p_z$ - states, while the topmost in GaN has the heavy holes with $p_x$ - like and $p_y$ - like states, where the axis z is directed along the hexagonal axis.

Therefore, the emission from high (low) Al - content Al$_x$Ga$_{1-x}$N is polarized along (perpendicular to) the c axis.

Recently many studies are focusing on the potential application of nanostructures, such as photonic crystal structures, nanoholes, nanodots and nanorods. In the studies of technology of photonic band gap suggest that in the case of dielectric rod nanoarrays or nanocolumns a large gap is opened for TM mode but not TE mode. Thus in the application this kind of structures for laser application is found the light source for TM mode.

In the c - plane InGaN/GaN quantum well systems the compressive strain is induced in the active layer and the polarization properties of light are TE polarized. Furthermore, there is a strong internal electric field caused by the spontaneous and piezoelectric polarization charge at the interfaces of the c-plane InGaN/GaN quantum well. This phenomenon leads to the quantum confined Stark effect, decreases the internal quantum efficiency and leads to the emission spectrum which is redshifted.

There are studies investigated the interface polarization charge, which use alloy materials to make better the performance. Many studies have focused on the nonpolar and semipolar planes. These results have testified that the light emission will be polarized, and quantum confined Stark effect will be reduced. However due to higher cost for the a - plane and m - plane substrates, it would be better to use the c - plane substrate. In the work the c - plane InGaN/AlGaN quantum well structure instead of the InGaN/GaN quantum well in order to obtain the tensile strain in the quantum well layer is considered. In previous studies and calculations have been shown that in nitride materials the $|Z\rangle$ - like state is generated when quantum well layer is under a tensile biaxial strain.

Besides the nitride-based devices, also group-II oxides have been considered for both highly efficient laser diodes and high performance field effect transistors. The induced piezoelectric field plays a significant role for both band structure and optical gain. However, the orientation of the crystal structure significantly modifies the band structure through strain effect. It has been proved experimentally that growth along crystal directions different from the [0001] direction leads to an increase in the quantum efficiency by decreasing the strain induced electric field in the quantum well region, possibly leading to the ways of obtaining highly efficient white laser diodes. There have been theoretical works studying the effects of crystal orientation on the piezoelectric field in strained wurtzite quantum well. However the piezoelectric effect consists not only of a strain induced polarization it also takes into consideration response of the electric field and polarization on the strain. These effects are studied in the paper.

A deeper understanding of an influence of band structures on an optical properties should help to answer on many questions. In addition in these materials the interesting effects of strong electron-hole Coulomb interaction are presented. Many-body interactions lead to effects, which consist screening, dephasing, bandgap renormalization and phase-space filling.

The paper is organized as follows. In the section 2 we present the microscopic many-body theory which based on the semiconductor Bloch equations that is Heisenberg equations for optical polarization and carriers populations. In the section 3 we consider the quantum well, which is oriented perpendicular to the growth direction (0001). We research overlap integral of electron and hole wave functions, calculate the exciton binding energy in the quantum well. We calculate Hartree and Hartree-Fock gain spectrum. We calculate exciton absorption spectra in the wurtzite quantum
well and compare its with the absorption spectra in quantum well with parabolic bands. We calculate Hartree and Hartree-Fock renormalization energy spectra. The red shift of the gain spectra caused by an electron-electron and hole-hole Coulomb interaction. A significant Sommerfeld enhancement is calculated. This enhancement of the electric dipole moment caused by an electron-hole Coulomb interaction of attraction.

B. Hartree-Fock problem of electron-hole pair in GaN quantum well

To make the analysis as simple as possible we assume a nondegenerate situations described by the Hamiltonian \( \hat{H} = \hat{H}_0 + \hat{V} + \hat{H}_{\text{int}} \), which consists in the electron-hole representation of the kinetic energy of an electron \( \epsilon_{\nu\alpha}^e \), and the kinetic energy of a hole \( \epsilon_{\nu\alpha}^h \):

\[
\hat{H}_0 = \sum_{\nu} \epsilon_{\nu\alpha}^e \hat{a}_{\nu\alpha}^+ \hat{a}_{\nu\alpha} + \epsilon_{\nu\alpha}^h \hat{b}_{\nu\alpha}^+ \hat{b}_{\nu\alpha},
\]

where \( \nu \) is a transversal in-plane of the quantum well carriers quazimomentum, \( \hat{a}_{\nu\alpha}^+ \), \( \hat{a}_{\nu\alpha} \), \( \hat{b}_{\nu\alpha}^+ \), \( \hat{b}_{\nu\alpha} \) are the annihilation and creation operators of electron and hole. Coulomb interaction Hamiltonian for a particles in the electron-hole representation is written in the form:

\[
\hat{V} = \frac{1}{2} \sum_{\nu\alpha} V_{\nu\alpha} \hat{a}_{\nu\alpha}^+ \hat{a}_{\nu\alpha}^+ \hat{a}_{\nu\alpha}^+ \hat{a}_{\nu\alpha} + V_{\nu\alpha} \hat{b}_{\nu\alpha}^+ \hat{b}_{\nu\alpha}^+ \hat{b}_{\nu\alpha}^+ \hat{b}_{\nu\alpha} - 2 V_{\nu\alpha} \hat{a}_{\nu\alpha}^+ \hat{b}_{\nu\alpha}^+ \hat{a}_{\nu\alpha} \hat{b}_{\nu\alpha},
\]

where

\[
V_{\nu\alpha} = \frac{x^2}{2} \int_{-w/2}^{+w/2} d\nu \int_{-w/2}^{+w/2} d\nu' \chi_{\nu\alpha}(z) \chi_{\nu\alpha'}(z') \frac{2\pi}{q} e^{-|\nu-z|} \chi_{\nu\alpha}(z),
\]

is Coulomb potential of the quantum well, \( \varepsilon \) - is a permittivity of host material of the quantum well, \( A \) - is a area of the quantum well in the \( xy \) plane.

The Hamiltonian of the dipole interaction with electromagnetic field is described as follows

\[
\hat{H}_{\text{int}} = -\frac{1}{\hbar} \sum_{\nu\alpha} \nu_{\alpha} \hat{p}_{\nu\alpha} E^* e^{i\omega t} + (\hat{p}_{\nu\alpha}^*)^+ E e^{-i\omega t},
\]

where

\[
\hat{p}_{\nu\alpha} = \langle \hat{b}_{\nu\alpha} \hat{a}_{\nu\alpha} \rangle - \langle \hat{b}_{\nu\alpha} \rangle \langle \hat{a}_{\nu\alpha} \rangle \]

is a microscopic dipole due to an electron-hole pair with electron (hole) momentum \( \nu \) (-\( \nu \)) and subband label \( \nu \). \( \hat{p}_{\nu\alpha} = \int d\mu U_{j',\nu\alpha}^* \hat{\mathbf{p}} U_{j\nu\alpha} \) - is the matrix element of the electric dipole moment, which depends from the wave vector \( \mathbf{k} \) and subband label between which occur direct interband transitions, \( e \) - is an unit vector of the vector potential of an electromagnetic wave, \( \mathbf{p} \) - is a momentum operator. Subbands are described wave functions \( U_{j\nu\alpha} \). \( j', \nu' \) - is a number of subband from the conduction band, \( j\nu \) - is an electron spin, \( j', \nu' \) - is a number of subband from the valence band, \( \sigma \) -is a hole spin. We consider the first lowering subband of conduction \( j' = 1 \) and first topmost valence subband \( j = 1 \). \( E \) and \( \omega \) - are an electric field amplitude and frequency of an optical wave.

We enter the approach which simplifies calculations in a solving problem about an electron-hole gas that is consider the problem in the case high density of an electron-hole gas (case \( r_s < 1 \)). The estimating the ratio of Coulomb potential energy to Fermi energy is found,

\[
r_s = \frac{E_C}{E_F} = \frac{2mc^2}{\varepsilon \hbar^2 \sqrt{\pi n}} = 0.73,
\]

for the concentrations of an electron-hole gas \( n = 10^{12} \text{cm}^{-2} \), the material permittivity \( \varepsilon = 9.38 \), the transversal effective mass of electron at \( \Gamma \) point \( m = 0.18 \) (inverse 2-th derivative of an energy from a transversal wave vector). This indicates that the Fermi energy dominates with respect to Coulomb potential energy at \( r_s \to 0 \). That is with the increasing density it increases rapidly than the Coulomb energy and at \( r_s \to 0 \) dominate the terms which correspond a cyclic diagrams.

Heisenberg equation for a electron \( \hat{n}_{\nu\alpha}^e = (\hat{a}_{\nu\alpha}^+ \hat{a}_{\nu\alpha}) \) and hole \( \hat{n}_{\nu\alpha}^h = (\hat{b}_{\nu\alpha}^+ \hat{b}_{\nu\alpha}) \) populations is written in the form:

\[
\frac{\partial \hat{n}_{\nu\alpha}^e}{\partial t} = \frac{i}{\hbar} [\hat{H}, \hat{n}_{\nu\alpha}^e].
\]
Figure 2. (Color online) Calculated Hartree-Fock absorption spectra for quantum well of width of 2 nm at concentration of carriers $n = p = 5 \times 10^{11}$ cm$^{-2}$ (Curve 1), $n = p = 10^{11}$ cm$^{-2}$ (Curve 2), $n = p = 0$ cm$^{-2}$ (Curve 3) at temperature 300 K.

Figure 3. (Color online) Hartree gain spectrum (Curve 2), Hartree-Fock gain spectrum (Curve 1) at the concentration of carriers $n = p = 9 \times 10^{12}$ cm$^{-2}$ for quantum well of width of 2 nm at the temperature 300 K.

Substituting (1), (2), (4) in (6), is obtained:

$$\hbar \frac{\partial \hat{n}_{\nu e}^{\psi \psi}}{\partial t} = -2Im[\mu_{p}^{\nu e} E(t)\langle \hat{\psi}_{p}^{\nu e} \rangle^*] + \sum_{q} V(q) \times \left( \langle \hat{a}^{+}_{p+q-k} \hat{a}^{+}_{k} \hat{a}^{+}_{p-q-k} \hat{a}^{+}_{p} \rangle - \langle \hat{a}^{+}_{p+q-k} \hat{h}^{+}_{k} \hat{a}^{+}_{p-q-k} \hat{a}^{+}_{p} \rangle - \langle \hat{a}^{+}_{p+q-k} \hat{h}^{+}_{k} \hat{a}^{+}_{p-q-k} \hat{a}^{+}_{p} \rangle \right).$$  \hfill (7)

Factorizing the convolutions of operators with the help of Wick theorem, Heisenberg equation for an electron population is obtained:

$$\hbar \frac{\partial \hat{n}_{\nu e}^{\psi \psi}}{\partial t} = -2Im[\mu_{p}^{\nu e} E(t)] + \sum_{q} V(q)\langle \hat{\psi}_{p+q}^{\nu e} \rangle^*].$$  \hfill (8)

The pairwise convolutions originate from the $\psi$ operators which taken in different points because this approach is Hartree-Fock one.
In the second order respecting Coulomb potential energy

\[ \frac{\hbar}{\partial t} \hat{n}^{\text{rem}}_p = -\sum_{k,q} 2\pi V^2(q) D(\epsilon_c(p) + \epsilon_c(k+q) - \epsilon_c(k) - \epsilon_c(p+q)) \times \hat{n}^p_{k+q}(1 - \hat{n}^p_{k}) \times \hat{n}^q_{p+q}(1 - \hat{n}^q_{p+q}) \hat{n}^p_{k+q} \hat{n}^q_{p+q} \times \hat{n}^p_{k+q}(1 - \hat{n}^p_{k}) \times \hat{n}^q_{p+q}(1 - \hat{n}^q_{p+q}) \hat{n}^p_{k+q} \hat{n}^q_{p+q} \times \hat{n}^p_{k+q}(1 - \hat{n}^p_{k}) \times \hat{n}^q_{p+q}(1 - \hat{n}^q_{p+q}) \hat{n}^p_{k+q} \hat{n}^q_{p+q}, \]  

(9)

where \( D(\Delta) = \delta(\Delta) - i\pi^{-1} P(\Delta) \), and \( P \) denotes principal value.

We assume that

\[ \frac{\partial \hat{n}^{\text{rem}}_p}{\partial t} = \frac{\partial \hat{n}^{\text{rem}}_p}{\partial t} = 0. \]  

(10)

One can find the expectation value from the convolution of two operators: \( \langle \hat{a}^+_k \hat{a}_p(\tau) \rangle \) regarding the density matrix, i.e. the some statistic operator \( \rho = \frac{e^{\beta \hat{H}_0}}{tr(e^{\beta \hat{H}_0})} \). In the interaction representation \( \hat{a}_p(\tau) = e^{-\tau \hat{H}_0} \hat{a}_p e^{\tau \hat{H}_0} \), where \( \hat{H}_0 = \sum_p \epsilon^p \hat{a}^+_p \hat{a}_p \). Let us write Heisenberg equation for \( \langle \hat{a}^+_k \hat{a}_p(\tau) \rangle \):

\[ \frac{d}{d\tau} \langle \hat{a}^+_k \hat{a}_p(\tau) \rangle = \epsilon^p \langle \hat{a}^+_k \hat{a}_p(\tau) \rangle. \]  

(11)

The solution of which is written in the form:

\[ \langle \hat{a}^+_k \hat{a}_p(\tau) \rangle = e^{\tau \epsilon^p} \langle \hat{a}^+_k \hat{a}_p \rangle. \]  

(12)

Without loss of generality we assume \( \tau = \beta \). Then the left side of equation (12) can be rewritten in the form \( \frac{S_p(e^{\beta \hat{H}_0} \rho e^{\beta \hat{H}_0})}{S_p(e^{\beta \hat{H}_0})} = \langle \hat{a}_p \hat{a}^+_k \rangle \). Using the proved equality the equation (12) can be rewritten:

\[ \langle \hat{a}_p \hat{a}^+_k \rangle = e^{\beta \epsilon^p} \langle \hat{a}^+_k \hat{a}_p \rangle. \]  

(13)

Since for fermions \( \hat{a}_p \hat{a}^+_k = \delta_{pk} - \hat{a}^+_k \hat{a}_p \), from equation (13) the expression for the electron population through Fermi distribution function is obtained:

\[ \langle \hat{a}^+_k \hat{a}_p \rangle = \frac{1}{1 + e^{\beta \epsilon^p}}, \]  

(14)

where \( \epsilon^p = \epsilon^p - E_F \), \( E_F \) - Fermi energy.

In calculations of the sum in the ground state energy of electron gas in the second order with respect to Coulomb potential energy can obtain

\[ \epsilon^{(2)} = m \sum_{k_1, k_2 < k_F} \sum_{k_3, k_4 > k_F} \frac{(12V^4(14V^4)(34V^2(12))}{p_1^2 + p_2^2 + p_3^2 + p_4^2} \]  

(15)

Since \( p_1^2 + p_2^2 - p_3^2 - p_4^2 = 2q^2 + 2q(p_2 - p_1) \), then

\[ \epsilon^{(2)} = -m a(4\pi e^2)^2 \left( \frac{\Omega}{(2\pi)^2} \right)^3 \int d^3q \int d^3p_1 \int d^3p_2 \]  

\[ \times 2^4(q + q(p_2 - p_1)), \]  

the coefficient before integrals may be written as follows

\[ \frac{1}{N} \left( \frac{4\pi}{(2\pi)^2} \right)^2 \left( \frac{\Omega}{(2\pi)^2} \right)^3 \frac{3\pi^2 N^2}{2^2} \]  

(17)

in Ry/electron the formula (16) may be rewritten

\[ \epsilon^{(2)} = - \frac{3}{8\pi^2} \int \frac{d^3q}{q} \int \frac{d^3p_1}{p_1} \quad \text{if} \quad p_1 \leq 1 \]  

\[ \quad \times \int \frac{d^3p_2}{p_2} \quad \text{if} \quad p_2 \leq 1, \]  

(18)
where $\Omega$ - is the volume of the crystal, $\frac{\Omega}{(2\pi)^{3}}$ - is the density of state in k space, $N = \frac{\Omega}{(2\pi)^{3}}k_{F}^{3}$. And exchange correlation energy:

$$
\epsilon^{(2)} = -\frac{3}{16\pi^{2}} \int \frac{d^{3}q}{q^{2}} \int \frac{d^{3}p_{1}}{p_{1} > 1} \frac{d^{3}p_{2}}{|p_{2} + q| > 1} \times \int \frac{d^{3}p_{3}}{|p_{3} + q| > 1} \frac{d^{3}p_{4}}{|p_{4} + q| > 1} \times \frac{1}{q^{2} + q(p_{2} - p_{1}) q^{2} + q(p_{3} - p_{1}) q^{2} + q(p_{4} - p_{1})},
$$

(19)

In the third order regarding Coulomb potential energy:

$$
\epsilon^{(3)} = 2(\frac{\alpha_{e}}{\pi})(\frac{3}{8\pi^{2}}) \int \frac{d^{3}q}{q^{2}} \int \frac{d^{3}p_{1}}{p_{1} > 1} \int \frac{d^{3}p_{2}}{|p_{2} + q| > 1} \int \frac{d^{3}p_{3}}{|p_{3} + q| > 1} \times \frac{1}{q^{2} + q(p_{2} - p_{1}) q^{2} + q(p_{3} - p_{1}) q^{2} + q(p_{4} - p_{1})},
$$

(20)

$$
\epsilon^{(3)} = 2(\frac{\alpha_{e}}{\pi})(\frac{3}{8\pi^{2}}) \int \frac{d^{3}q}{q^{2}} \int \frac{d^{3}p_{1}}{p_{1} > 1} \int \frac{d^{3}p_{2}}{|p_{2} - p_{1}|} \int \frac{d^{3}p_{3}}{|p_{3} - p_{1}|} \times \frac{1}{q^{2} + q(p_{2} - p_{1}) q^{2} + q(p_{3} - p_{1})},
$$

(21)

$$
\epsilon^{(3)} = 2(\frac{\alpha_{e}}{\pi})(\frac{3}{8\pi^{2}}) \int \frac{d^{3}q}{q^{2}} \int \frac{d^{3}p_{1}}{p_{1} > 1} \int \frac{d^{3}p_{2}}{|p_{2} - p_{1}|} \int \frac{d^{3}p_{3}}{|p_{3} - p_{1}|} \times \frac{1}{q^{2} + q(p_{2} - p_{1}) q^{2} + q(p_{3} - p_{1})},
$$

(22)

$$
\epsilon^{(3)} = r_{e}(A^{(3)} \int \frac{d^{3}q}{q^{2}} + B^{(3)} \int \frac{d^{3}q}{q^{2}} + C^{(3)} \int \frac{d^{3}q}{q^{2}}),
$$

(23)

where

$$
\alpha = (\frac{4}{9\pi})^{1/3},
$$

(24)

the constants $A^{(3)}$, $B^{(3)}$, $C^{(3)}$ are defined by integrals:

$$
A^{(3)} = 2(\frac{\alpha_{e}}{\pi})(\frac{3}{8\pi^{2}})(2\pi)^{3}p_{F}^{3} \int_{0}^{1} d\xi_{1} \int_{0}^{1} d\xi_{2} \int_{0}^{1} d\xi_{3} \times \frac{1}{(\xi_{1} + \xi_{2})(\xi_{1} + \xi_{3})},
$$

$$
B^{(3)} = 2(\frac{\alpha_{e}}{\pi})(\frac{3}{8\pi^{2}})(2\pi)^{3}p_{F}^{3} \int_{0}^{1} d\xi_{1} \int_{0}^{1} d\xi_{2} \int_{0}^{1} d\xi_{3} \times \frac{1}{(\xi_{1} + \xi_{2})(\xi_{1} + \xi_{3})},
$$

$$
C^{(3)} = 2(\frac{\alpha_{e}}{\pi})(\frac{3}{8\pi^{2}})(2\pi)^{3} \int_{0}^{1} d\xi_{1} \int_{0}^{1} d\xi_{2} \int_{0}^{1} d\xi_{3} \times \frac{1}{(\xi_{1} + \xi_{2})(\xi_{1} + \xi_{3})},
$$

(25)

Detailed analysis all integrals testifies that in the each order regarding Coulomb potential energy $r_{e}$ appears in the capacity of multiplier in the contributions all diagrams with the exception of cyclic ones. Because the latter become apparent the dominate at summation all diagrams in the limiting case of high density of electron-hole gas at $r_{e} \to 0$.

For calculations of the sum in the energy of the ground state of an electron gas in all orders of the perturbation theory in the article 64 as the propagator function is entered:

$$
F_{q}(t) = \int d^{3}pe^{-|t|^{2}(\frac{1}{2}\gamma^{2} + q\eta)},
$$

(26)

and his Fourier transform:

$$
Q_{q}(u) = \int d^{3}p \int_{-\infty}^{\infty} e^{iuq}e^{-|t|\frac{1}{2}(q^{2} + q\eta)}dt.
$$

(27)

In works 64–66 the direct correspondence between the diagrams of a given order and the integrals is found, Fourier
transformations of which are equal:

\[ A_n = \frac{q}{2\pi} \int_{-\infty}^{\infty} du [Q_q(u)]^n. \]  

(28)

The complete contribution of all cyclic diagram in n-order of the perturbation theory are shown to be defined through Fourier transform as follows \(^{64-66}\):

\[
\epsilon' \equiv \epsilon^{(2)} + \epsilon^{(3)} + \epsilon^{(4)} + \ldots
\]

\[ = -\frac{3}{8\pi} \int \frac{dq}{q^2} \frac{1}{2\pi} \sum_{n=2}^{n} [(\hat{F}, \hat{V}, \ldots \hat{V})]^{(n-1)} \int_{-\infty}^{\infty} du \left(\frac{1}{n} [Q_q(u)]^{n}(\frac{2\pi q}{\hbar^2})^{n-2}\right) \]

\[ \times \sum_{n=2}^{n-1} \frac{(-1)^{n-1}}{n}[\hat{f}]^{n-1}[Q_q(u)]^{n}(\frac{2\pi q}{\hbar^2})^{n-2}, \]

(29)

where we choose \( \hat{F} \) from the sum of four operators from equation (9), which consist of four products of operators of creation and annihilation particles, for instance: \( \hat{F} = \hat{a}^+_p \hat{a}^-_{k-q} \hat{a}^-_{p-q} \hat{a}^+_k \), then we obtain

\[ \hat{f} = \hat{n}_p \hat{n}_k + (1 - \hat{n}_p + q)(1 - \hat{n}_k). \]  

(30)

In this section we derive the equation of motion for the exceptional value of the product \( \hat{b}^-_p \hat{a}_p \), of a microscopic dipole which specifies of a medium polarization which becomes macroscopic due to an applied external field.

The average value of a certain physical magnitude \( \hat{F} \), which responds the operator \( \hat{F} \) can be expressed through the spur of matrix, a certain statistic operator for which Heisenberg equation is satisfied:

\[ \langle \hat{F} \rangle = \text{Sp}(\hat{w}_0 \hat{F}) + \frac{2\pi}{\hbar} D(-\epsilon_{p,-q} + \epsilon_{p,-q} + \epsilon_{p,-q} + \epsilon_{p,+}) \text{Sp}([\hat{F}, \hat{V}_0] \hat{w}_0), \]

(31)

where \( \hat{w}_0 = \frac{e^{-\hat{H}_0/\kappa T}}{Sp(e^{-\hat{H}_0/\kappa T})} \), that is the density matrix \( \hat{w}_0 \) is assumed to be described the canonical distribution of Gibbs; in interaction representation the time dependence as a wave function thus a some operator may be expressed through the Hamiltonian of the system of noninteraction particles: \( \hat{V}_0 = e^{\text{H}_0 t/\hbar} V e^{-\text{H}_0 t/\hbar}. \)

Heisenberg equation for the described system of an electron-hole gas takes on form:

\[
\frac{d\hat{a}^{\nu_k\nu_h}}{dt} = -\hat{a}^{\nu_k\nu_h} \hat{P}^{\nu_k\nu_h} - i \sum_{\nu} \hat{V}^{\nu_k\nu_h} \left(-1 + \hat{n}^{\nu_h}_p + \hat{n}^{\nu_k}_p\right) + i \left(\sum_{\nu,\nu} V^{\nu_k\nu_h,\nu_k\nu_h} \left(\hat{a}^{\nu_k+}_{k+q} \hat{a}^{\nu_h+}_{p+q} \hat{b}^-_{k+q} \hat{b}^-_{p+q} \hat{a}^-_{k} \hat{a}^-_{p}\right) + V^{\nu_k\nu_h,\nu_k\nu_h} \left(\hat{b}^{\nu_k+}_{k+q} \hat{b}^{\nu_h+}_{k+q} \hat{b}^-_{k+q} \hat{b}^-_{k+q} \hat{a}^-_{k} \hat{a}^-_{p}\right) \right) \]

\[ - \sum_{\nu,\nu} V^{\nu_k\nu_h,\nu_k\nu_h} \left(\left(\hat{a}^{\nu_k+}_{k+q} \hat{a}^{\nu_h+}_{p+q} \hat{b}^-_{k+q} \hat{a}^-_{k} \hat{a}^-_{p}\right) + \left(\hat{b}^{\nu_k+}_{k+q} \hat{b}^{\nu_h+}_{k+q} \hat{b}^-_{k+q} \hat{b}^-_{k+q} \hat{a}^-_{k} \hat{a}^-_{p}\right) \right) \]  

(32)

Figure 4. (Color online) Calculated energy spectra for the heavy (hh1), light (lh1) holes for the nonoccupied valence band (Curve 5, Curve 6), Hartree energy spectra for the heavy (hh2), light (lh2) holes (Curve 1, Curve 2) and Hartree-Fock energy spectra for the heavy (hh3), light (lh3) holes (Curve 3, Curve 4) for the quantum well with width 2 nm at concentration of carriers \( n = p = 9 \times 10^{12} \text{ cm}^{-2} \) at temperature 300 K.
where $\omega_{p}^{h,\nu_{h}} = \frac{1}{\hbar}(\epsilon_{p} + \epsilon_{h}^{p} + \epsilon_{h}^{q})$, $\Omega_{p}^{h,\nu_{h}} = \frac{1}{\hbar}p^{h,\nu_{h}} E e^{-i\omega t}$. Using an operator algebra and a formalism of density matrix can be obtained the following expressions:

$$
\frac{d\rho_{p,q}^{h,\nu_{h}}}{dt} = -i\omega_{p}^{h,\nu_{h}} \rho_{p,q}^{h,\nu_{h}} - i\Omega_{p}^{h,\nu_{h}} \left(-\hat{n}_{p}^{\nu_{h}} + \hat{n}_{p}^{\nu_{h}}\right) - i\sum_{q} W_{p,q}^{\nu_{h}^{p},\nu_{h}^{q}} \left(\hat{\rho}_{p,q}^{\nu_{h}^{p},\nu_{h}^{q}} + \hat{\rho}_{p,q}^{\nu_{h}^{q},\nu_{h}^{p}}\right) + \frac{i}{\hbar} \sum_{\alpha = e,h} \sum_{\nu_{\alpha},\nu_{\beta}} \sum_{k,q} W_{q}^{\nu_{\alpha}^{k},\nu_{\beta}^{q}} W_{p,q}^{\nu_{\alpha}^{p},\nu_{\beta}^{q}} \delta_{\alpha,\beta} \epsilon_{p}\epsilon_{q} = \epsilon_{p}
$$

(33)

The equation (33) describes the oscillation of the polarization at the transition frequency also the stimulated emission or absorption processes. In a capacity of the population functions we choose Fermi distribution functions. The transition frequency $\omega_{p}^{h,\nu_{h}}$ is derived as follows:

$$
\omega_{p}^{h,\nu_{h}} = \frac{1}{\hbar}(\epsilon_{p} + \epsilon_{h}^{p} + \epsilon_{h}^{q}) + i\sum_{\alpha = e,h} \sum_{\nu_{\alpha},\nu_{\beta}} \sum_{k,q} \left(W_{q}^{\nu_{\alpha}^{k},\nu_{\beta}^{q}} \left(-\hat{n}_{k}^{\nu_{h}}\right) + W_{q}^{\nu_{\alpha}^{p},\nu_{\beta}^{q}} \left(-\hat{n}_{p}^{\nu_{h}}\right)\right) + \delta_{\alpha,\beta} \epsilon_{p}\epsilon_{q} = \epsilon_{p}
$$

(34)

Functions $\hat{\rho}_{p,q}^{\nu_{h}^{p},\nu_{h}^{q}}$ and $\hat{\rho}_{p,q}^{\nu_{h}^{q},\nu_{h}^{p}}$ are defined as follows:

$$
\hat{\rho}_{p,q}^{\nu_{h}^{p},\nu_{h}^{q}} = i \sum_{k} W_{q}^{\nu_{h}^{k},\nu_{h}^{q}} - W_{k+p,q}^{\nu_{h}^{p},\nu_{h}^{q}} D(-\hat{n}_{p}^{\nu_{h}} - \hat{n}_{k}^{\nu_{h}} + \hat{n}_{k}^{\nu_{h}})(\hat{n}_{k}^{\nu_{h}} - \hat{n}_{p}^{\nu_{h}}) \hat{n}_{p}^{\nu_{h}} + (1 - \hat{n}_{p}^{\nu_{h}}) \hat{n}_{k}^{\nu_{h}}(1 - \hat{n}_{p}^{\nu_{h}}),
$$

(35)

$$
\hat{\rho}_{p,q}^{\nu_{h}^{q},\nu_{h}^{p}} = i \sum_{k} W_{k+q,p}^{\nu_{h}^{p},\nu_{h}^{q}} - W_{q}^{\nu_{h}^{p},\nu_{h}^{q}} D(-\hat{n}_{p}^{\nu_{h}} - \hat{n}_{k}^{\nu_{h}} + \hat{n}_{k}^{\nu_{h}})(\hat{n}_{k}^{\nu_{h}} - \hat{n}_{p}^{\nu_{h}}) \hat{n}_{p}^{\nu_{h}} + (1 - \hat{n}_{p}^{\nu_{h}}) \hat{n}_{k}^{\nu_{h}}(1 - \hat{n}_{p}^{\nu_{h}}),
$$

(36)

We have replaced the bare Coulomb potential energy with the screened one:

$$
V_{q}(1 - VM + (VM)^{2} - (VM)^{3} + ...),
$$

(37)

where

$$
M = \sum_{k} \frac{n(e_{k} + q) - n(e_{k})}{e_{k} + q - e_{k}}.
$$

(38)

The coefficient before the sum in the second term of the sequence (37) is equal

$$
N \frac{m}{2\pi^{3}} (\frac{4\pi e^{2}}{4\pi})^{2} \frac{\Omega}{(3\pi)^{2}} \frac{1}{k_{p}^{2}} = N \frac{m e^{4}}{2\pi^{3}} (\frac{4\pi e^{2}}{4\pi})^{2} \frac{\Omega}{(3\pi)^{2}} \frac{1}{k_{p}^{2}} = \frac{n e^{4}}{2\pi^{3}} \frac{4}{3\pi},
$$

(39)

in the third term of the sequence:

$$
\frac{m^{2}}{2\pi^{3}} (\frac{4\pi e^{2}}{4\pi})^{2} \frac{\Omega}{(3\pi)^{2}} \frac{1}{k_{p}^{2}} = \frac{n e^{4}}{2\pi^{3}} \frac{4}{3\pi} a_{r},
$$

(40)

Then the sequence may be rewritten in the form indefinitely decreased geometric progression

$$
\frac{1}{\eta} = \frac{4}{3\pi} \int d^{3}k \frac{1}{\eta} \frac{n(e_{k} + q) - n(e_{k})}{(k_{1} + q)^{2}} + \frac{4}{3\pi} a_{r} \int d^{3}k_{1} d^{3}k_{2} \frac{1}{\eta} \frac{n(e_{k_{1} + q} - n(e_{k_{1}})}{(k_{1} + q)^{2} - k_{1}^{2}} \frac{n(e_{k_{2}} - n(e_{k_{2}})}{(k_{2} + q)^{2} - k_{2}^{2}} - ...
$$

(41)

Under summation all terms of the sequence one obtain:

$$
W_{q}^{\nu_{h}^{p},\nu_{h}^{q}} = \frac{V_{q}^{\nu_{h}^{p},\nu_{h}^{q}}}{\epsilon_{q}(N)}
$$

(42)

For the dielectric function we use the static Lindhard formula:

$$
\epsilon_{q}(N) = 1 + \sum_{\rho = e,h} \sum_{\nu_{\rho}} \sum_{p} V_{q}^{\nu_{\rho}^{p},\nu_{\rho}^{q}} \frac{\hat{n}_{p}^{\nu_{h}} - \hat{n}_{p}^{\nu_{h}^{p}}}{\epsilon_{p}^{\nu_{h}^{p}} - \epsilon_{p}^{\nu_{h}}}
$$

(43)
Since the cyclic diagrams are a primary type of diagram in a scattering process at the high density of an electron-hole gas than in this case the diagram method is equivalent of the self-consistency method as well as the random phase approximation.

The answer how to derive the integro-differential equation (33) for a microscopic dipole is following scheme:

\[
\omega_p^{\nu e_h} : \hat{V}_q^{\nu e_h \nu e_h} \to W_q^{\nu e_h \nu e_h \nu e_h}, \quad \hat{n}_{p+q}^{\nu e_h} \to \Xi_{p+q}^{\nu e_h}
\]

(44)

plus the expression the schematic representation of which in the form of a binary blister,

\[
\sum_p \frac{d\hat{n}_{p+q}^{\nu e_h}}{dt} : \hat{V}_q^{\nu e_h \nu e_h \nu e_h} \to W_q^{\nu e_h \nu e_h \nu e_h}, \quad \hat{n}_{p}^{\nu e_h} \to \Xi_{p}^{\nu e_h}
\]

(45)

plus the expression the schematic representation of which in the form of an oyster.

The sum with respect to momentum in the polarization equation which takes to account the carrier-carrier correlations the higher orders than Hartree-Fock can be found if into the self energy in the equation to add the same term which is entered into the equation in Hartree-Fock approximation replacing therein Coulomb potential energy with the screened one, Fermi distribution functions - \(\Xi_{p+q}^{\nu e_h}\), functions, plus the expression, the schematic representation of which in the form of a binary blister. In the just integro-differential equation is added the same term which is entered into the equation in Hartree-Fock approximation replacing therein Coulomb potential energy with the screened one, Fermi distribution functions - \(\Xi_{p}^{\nu e_h}\) functions, plus the expression, the schematic representation of which in the form of an oyster. We consider the coupled closed diagrams. The sum of all uncoupled diagrams which include the k closed loops which have \(m_1, m_2, ..., m_q\) tops correspondingly is the sum of all closed diagrams of the m order.

The well-known in literature polarization equation is divided via diagonal and nondiagonal with respect to \(\hat{p}_p^{\nu e_h}\) terms

\[
\frac{d\hat{n}_{p}^{\nu e_h}}{dt} = -i\omega_p^{\nu e_h} \hat{n}_{p}^{\nu e_h} - i\Omega_p^{\nu e_h} (1 + \hat{n}_{p}^{\nu e_h} + \hat{n}_{p}^{\nu h}) + (\Gamma_p^{\nu_\alpha} + \Gamma_p^{\nu_\beta}) \hat{n}_{p}^{\nu e_h} + \sum_q (\Gamma_p^{\nu e_h} + \Gamma_p^{\nu h}) \hat{n}_{p+q}^{\nu e_h}.
\]

(46)

The transition frequency \(\omega_p^{\nu e_h}\) and Rabi frequency are derived as follows

\[
\omega_p^{\nu e_h} = \frac{1}{\hbar} (\varepsilon_{p}^{\nu e_h} + \varepsilon_{h}^{\nu e_h} + \Sigma_{\alpha=e,h} \sum_q \hat{V}_q^{\nu e_h \nu e_h \nu e_h} \hat{n}_{p+q}^{\nu e_h}),
\]

(47)

\[
\Omega_p^{\nu e_h} = \frac{1}{\hbar} (\varepsilon_{p}^{\nu e_h} E e^{-i\omega t} + \sum_q \hat{V}_q^{\nu e_h \nu e_h \nu e_h} \hat{n}_{p+q}^{\nu e_h}).
\]

(48)

Carrier-carrier correlations which lead to screening and dephasing are described the expressions which consist diagonal \(\hat{p}_p^{\nu e_h}\) terms and nondiagonal \(\hat{p}_p^{\nu e_h}\) terms contributions. For the diagonal contribution

\[
\Gamma_p^{\nu_\alpha} = \frac{1}{\pi} \sum_{\beta=e,h} \sum_{p+q} \sum_q (|\hat{W}_q^{\nu e_h \nu e_h \nu e_h}|^2 - \frac{1}{2} \delta_{\nu_\alpha \nu_\beta} W_{|q|\nu_\beta} W_{q \nu_\alpha \nu_\beta} W_{|p+q|\nu_\beta}) 
\times D(-\varepsilon_k^{\nu_\beta} - \varepsilon_k^{\nu_\alpha} + \varepsilon_{k-q}^{\nu_\beta} + \varepsilon_{k+q}^{\nu_\alpha}) \hat{n}_{k-q}^{\nu_\alpha} \hat{n}_{k+q}^{\nu_\beta} (1 - \hat{n}_{k-q}^{\nu_\alpha} \hat{n}_{k+q}^{\nu_\beta}).
\]

(49)

There are also nondiagonal contributions which couple the polarizations of different wave vectors and are defined from the expression:

\[
\Gamma_{p,q}^{\nu_\alpha} = \frac{1}{\pi} \sum_{\beta=e,h} \sum_{\nu_\beta \neq \nu_\alpha} \sum_{p+q} (|\hat{W}_q^{\nu e_h \nu e_h \nu e_h}|^2 - \hat{W}_{q \nu_\alpha \nu_\beta}^{\nu e_h \nu e_h} \hat{W}_{q \nu_\beta \nu_\alpha}^{\nu e_h \nu e_h} + \frac{1}{2} \delta_{\nu_\alpha \nu_\beta} W_{q \nu_\alpha \nu_\beta} W_{|q+q|\nu_\alpha} W_{|q+q|\nu_\beta})
\times D(-\varepsilon_k^{\nu_\alpha} - \varepsilon_k^{\nu_\beta} + \varepsilon_{k-q}^{\nu_\alpha} + \varepsilon_{k+q}^{\nu_\beta}) \hat{n}_{k-q}^{\nu_\beta} \hat{n}_{k+q}^{\nu_\alpha} (1 - \hat{n}_{k-q}^{\nu_\beta} \hat{n}_{k+q}^{\nu_\alpha}).
\]

(50)

We solve the differential equations system and derive algebraic equations system or the integral equation:

\[
\chi_p^{\nu e_h} = \frac{i}{\hbar} \pi (\frac{\hat{n}_{p}^{\nu e_h} + \hat{n}_{p}^{\nu h} - 1}{\omega_p^{\nu e_h}}) \frac{1}{\Gamma_p^{\nu e_h} + \Gamma_p^{\nu h}} (\mu^{\nu e_h}_{p} - \sum_q \hat{V}_q^{\nu e_h \nu e_h \nu e_h} \hat{n}_{p+q}^{\nu e_h} \frac{1}{|p+q|} \chi_{p+q}^{\nu e_h}).
\]

(51)

in which \(\omega_p^{\nu e_h}\) - is the self energy, that is the renormalized width of the band gap. The derived renormalization energy is the exchange energy. The sum \(\Gamma_p^{\nu e_h}\) defines the half-width of the exciton resonance. The polarization is expressed through the function \(\chi_p^{\nu e_h}\) as follows:

\[
\hat{p}_p^{\nu e_h} = \chi_p^{\nu e_h} E e^{-i\omega t}.
\]

(52)
The half-width of the gain spectra is calculated with the help of formulae:

\[
\Gamma_k^{\nu_0} = \frac{1}{2\pi} \sum_{\beta=e,h} \sum_{\nu_0} \int_0^{2\pi} d\varphi \int_0^{2\pi} d\alpha \int q dq \frac{1}{Q(\sum_{\nu_0} |\delta_{\nu_0}\rangle^{\nu_0}_{\nu_0} - \Gamma^{\nu_0}_{k+q})}(\sum_{\nu_0} |\delta_{\nu_0}\rangle^{\nu_0}_{\nu_0} - \Gamma^{\nu_0}_{k+q})^2
\]

\[
\times (\hat{n}_{k+q}^{\nu_0} (1 - \hat{n}_{k+q}^{\nu_0}) + (1 - \hat{n}_{k+q}^{\nu_0}) \hat{n}_{k+q}^{\nu_0} (1 - \hat{n}_{k+q}^{\nu_0})^2),
\]

(53)

\[
\Gamma_k^{\nu_0} = \frac{1}{2\pi} \sum_{\beta=e,h} \sum_{\nu_0} \int_0^{2\pi} d\varphi \int_0^{2\pi} d\alpha \int q dq \frac{1}{Q((\sum_{\nu_0} |\delta_{\nu_0}\rangle^{\nu_0}_{\nu_0} - \Gamma^{\nu_0}_{k+q})^2 - \frac{1}{2} \delta_{\nu_0}\nu_0 | \sum_{\nu_0} \int d\zeta \int dz \chi_{\nu_0}(z)\chi_{\nu_0}(z)' e^{-\nu_0(z-z') | \sum_{\nu_0} \int d\zeta \int dz \chi_{\nu_0}(z)\chi_{\nu_0}(z)' | \sum_{\nu_0} \int d\zeta \int dz \chi_{\nu_0}(z)\chi_{\nu_0}(z) |} | \sum_{\nu_0} \int d\zeta \int dz \chi_{\nu_0}(z)\chi_{\nu_0}(z)' |}
\]

\[
\times (\hat{n}_{k+q}^{\nu_0} (1 - \hat{n}_{k+q}^{\nu_0}) + (1 - \hat{n}_{k+q}^{\nu_0}) \hat{n}_{k+q}^{\nu_0} (1 - \hat{n}_{k+q}^{\nu_0})^2).\]

(54)

where \( Q = |k+q|, \varphi \)-is the angle between vectors \( k \) and \( q \). In calculations of the broadening caused carrier-carrier correlations one can see that in the schematic representations their expressions in the form of diagrams there are two expressions diagrams of the schematic representation of which in the form of an oyster and four expressions diagrams of the schematic representation of which in the form of a binary blister.

The polarization equation for the wurtzite quantum well in Hartree-Fock approximation with including the wave functions for an electron and hole written in the form 9.67.68, when the coefficients of development of the wave function for a hole dependence from wave vector in the basis of wave functions with the orbital angular momentum \( l = 1 \) and eigenvalue \( m_l \), his z component, known as spherical harmonics, one can look for as follows:

\[
\frac{d\hat{n}_{p}^{\nu_{0}}}{dt} = -i\omega_{p}^{\nu_{0}} \hat{n}_{p}^{\nu_{0}} - i\Omega_{p}^{\nu_{0}} (1 - \hat{n}_{p}^{\nu_{0}} + \hat{n}_{p}^{\nu_{0}})
\]

(55)

The transition frequency \( \omega_{p}^{\nu_{0}} \) and Rabi frequency with including the wave functions 9.67.68 are described in the form:

\[
\omega_{p}^{\nu_{0}} = \frac{1}{h}(\epsilon_{q0} + \epsilon_{p,h} - \sum q V_{q,nu_{0}nu_{0}}^{\nu_{0}} \hat{n}_{p+q}^{\nu_{0}} - \sum q V_{q,nu_{0}nu_{0}}^{\nu_{0}} \hat{n}_{p+q}^{\nu_{0}})
\]

(56)

\[
\Omega_{p}^{\nu_{0}} = \frac{1}{h}(\mu_{p}^{\nu_{0}} E e^{-i\omega t} + \sum q V_{q,nu_{0}nu_{0}}^{\nu_{0}} \hat{n}_{p+q}^{\nu_{0}})
\]

(57)

where

\[
V_{\nu_{0}nu_{0}nu_{0}}^{\nu_{0}} = \frac{1}{2} \sum_{\nu_{0}} \sum_{\nu_{0}} g_{\alpha} \int dq \int dz \chi_{\nu_{0}}(z)\chi_{\nu_{0}}(z)' | C_{p}^{\nu_{0}[m_{1},1]}V_{p}[m_{1},1]C_{Q_{1}}[n_{2},1]V_{Q_{1}}^{m_{2},1},
\]

(58)

\[
\sum_{\alpha} \sum_{\nu_{0}} g_{\alpha} V_{\nu_{0}nu_{0}nu_{0}}^{\nu_{0}} \hat{n}_{\nu_{0}p+q}^{\nu_{0}} = \frac{1}{2} \sum_{\nu_{0}} \sum_{\nu_{0}} g_{\alpha} \int dq \int dz \chi_{\nu_{0}}(z)\chi_{\nu_{0}}(z)' | C_{p}^{\nu_{0}[m_{1},1]}V_{p}[m_{1},1]V_{Q_{2}}^{m_{2},1}n_{\alpha},Q_{2},
\]

(59)

where \( \chi_{\nu_{0}}(z) \) - is envelope part of the quantum well wave functions, \( V_{p}[m_{1},1], C_{Q_{1}}^{m_{2},1} \) - are coefficients of the development of wave functions of a hole and electron at the envelope part, \( \varphi \)- is the angle between vectors p and q, \( g_{\alpha} \)- is a degeneracy order of a level.

The numerically solving this integro-differential equation can from Maxwell equations obtain the absorption coeffi-
C. Envelope wave vector formalism for conduction band and electron teleportation driven by magnetic field in dilute GaAsN quantum well

The Hamiltonian in the main axes of the effective mass tensor can be presented in the form:

\[
\hat{H} = \begin{pmatrix}
\sum_i \frac{k_i^2}{2 m_i} & \Delta \\
\Delta^* & \sum_i \frac{k_i^2}{2 m_i}
\end{pmatrix}
\begin{pmatrix}
|\frac{1}{2}, \frac{1}{2}\rangle \\
|\frac{1}{2}, -\frac{1}{2}\rangle
\end{pmatrix},
\]

(62)
Figure 7. (Color online) Calculated absorption spectra in a zinc-blende GaN/AlGaN quantum well at concentration of carriers $n = p = 0$ cm$^{-3}$ under the tensile biaxial strain (Curve 3), under the compressive biaxial strain (Curve 1) and for thin film GaN (Curve 2) for two-light polarization.

where $i = xx, yy, zz$. The Hamiltonian (62) is written in the basis of angular momentum $j = 1/2$ and magnetic quantum numbers $m_j = 1/2, -1/2$, which is related with $p$-like $\Gamma_4$ states by Clebsch-Gordan coefficients $36,69$:

$$
\begin{align*}
|1/2, 1/2\rangle & = 1/\sqrt{3} (|1, 0\rangle - \sqrt{2} |1, 1\rangle),
|1/2, -1/2\rangle & = 1/\sqrt{3} (|1, 0\rangle - \sqrt{2} |1, -1\rangle),
\end{align*}
$$

where $\alpha$=spin up, $\beta$=spin down.

In the new axes with effective mass $m^i = (m_{xx}^i m_{yy}^i m_{zz}^i)^{1/3}$ the hamiltonian may be rewritten in the form:

$$
\hat{H} = \sum_i \frac{\hbar^2}{2m^i} k_i^2 \Delta \sum_i \frac{\hbar^2}{2m^i} k_i^2 |\frac{1}{2}, 1/2\rangle
$$

(64)

The Hamiltonian (64) written in new values $x'_{xx} = x_{xx} (m_{xx}/m)^{1/2}$, $k'_{xx} = k_{xx} (m_{xx}/m)^{1/2}$. In the perpendicular magnetic field $H_z y$ the Hamiltonian can be presented

$$
\hat{H} = \begin{bmatrix} Q_1 \Delta & \Delta^* \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \end{bmatrix}.
$$

(65)

where

$$
Q_1 = \frac{\hbar^2}{2m^{xx}} ((k_x + \frac{eH_z y}{\hbar c})^2 + k_y^2 + k_z^2),
Q_2 = \frac{\hbar^2}{2m^{xx}} ((k_x + \frac{eH_z y}{\hbar c})^2 + k_y^2 + k_z^2).
$$

(66)

In the new axes $A'_{xx} = A_{xx} (m/m_{xx})^{1/2}$, $H'_{xx} = H_{xx} (m/m_{xx})^{1/2}$. We direct the axis $z''$ along magnetic field $H'$,

$$
H' = (\frac{m_{xx}}{m} H_{xx}^2 + \frac{m_{yy}}{m} H_{yy}^2 + \frac{m_{zz}}{m} H_{zz}^2)^{1/2},
$$

(67)

in the selected gauge of potential

$$
A'_{xx''} = H' y'', A'_{yy''} = 0, A'_{zz''} = 0.
$$

(68)

Schrödinger equation for virtual crystal GaAsN can be rewritten in the form:

$$
\begin{bmatrix} Q_1 - E \Delta \\ \Delta^* Q_2 - E \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \end{bmatrix} = 0.
$$

(69)

The solution of which can be found in expansion form with respect to Chebyshev-Hermitian polinoms

$$
\Psi = \Sigma_n C_n \exp^{-\xi^2/2} H_n(\xi),
$$

(70)

where $\int_{-\infty}^{+\infty} H_n(\xi) H_m(\xi) \exp^{-\xi^2} d\xi = 2^n n! \sqrt{\pi} \delta_{nm}$. Each term in expansion (9) defines wave function of Landau level
n if $\Delta = 0$. At $\Delta \neq 0$ it is pronounced the band mixing effect. If inserts new variables $\xi = s^{-1} \tilde{y}$, $\tilde{y} = y + y_0$, $y_0 = s^2 k_z$, $s^2 = \frac{h}{\mu c}$, that equations (69) can be presented of releasing oscillation center:

$$\begin{vmatrix} P_1 - E & \Delta \\ \Delta^* & P_2 - E \end{vmatrix} \begin{vmatrix} \Psi_1 \\ \Psi_2 \end{vmatrix} = 0,$$

(71)

where

$$\begin{align*}
P_1 &= \frac{h^2 s^{-2}}{2 m^{1/2}} (s^{-2} \tilde{y}^2 - \frac{\partial^2}{\partial \xi^2}) + \frac{h^2 k_z^2}{2 m^{1/2}}, \\
P_2 &= \frac{h^2 s^{-2}}{2 m^{1/2}} (s^{-2} \tilde{y}^2 - \frac{\partial^2}{\partial \xi^2}) + \frac{h^2 k_y^2}{2 m^{1/2}}.
\end{align*}$$

(72)

In the new variables $\xi$ the equation has the form:

$$\begin{vmatrix} R_1 - E & \Delta \\ \Delta^* & R_2 - E \end{vmatrix} \begin{vmatrix} \Psi_1 \\ \Psi_2 \end{vmatrix} = 0,$$

(73)

where

$$\begin{align*}
R_1 &= \frac{h^2 s^{-2}}{2 m^{1/2}} (\xi^2 - \frac{\partial^2}{\partial \xi^2}) + \frac{h^2 k_z^2}{2 m^{1/2}}, \\
R_2 &= \frac{h^2 s^{-2}}{2 m^{1/2}} (\xi^2 - \frac{\partial^2}{\partial \xi^2}) + \frac{h^2 k_y^2}{2 m^{1/2}}.
\end{align*}$$

(74)

Substitute the solution (70) in equation (73)

$$\begin{vmatrix} R_1 - E & \Delta \\ \Delta^* & R_2 - E \end{vmatrix} \begin{vmatrix} \Sigma_n C_1^1 \Psi_n(\xi) \\ \Sigma_n C_2^1 \Psi_n(\xi) \end{vmatrix} = 0,$$

(75)

where $\Psi_n(\xi) = \exp^{-\xi^2/2} H_n(\xi)$. By multiplying in the left side the equation on harmonic oscillation function and integrating with respect to variable $\xi$ by all space can obtain

$$\begin{vmatrix} S_1 - E_n & \Delta \\ \Delta^* & S_2 - E_n \end{vmatrix} \begin{vmatrix} C_1^1 \\ C_n^2 \end{vmatrix} = 0,$$

(76)

where

$$\begin{align*}
S_1 &= \frac{h^2 s^{-2}}{2 m^{1/2}} (n + 1/2) + \frac{h^2 k_z^2}{2 m^{1/2}}, \\
S_2 &= \frac{h^2 s^{-2}}{2 m^{1/2}} (n + 1/2) + \frac{h^2 k_y^2}{2 m^{1/2}}.
\end{align*}$$

(77)

From (76) the energy spectrum the quantization Landau levels:

$$\begin{align*}
E_{n,\pm} &= \frac{1}{2} \left( \frac{h^2 s^{-2}}{\mu} (n + 1/2) + \frac{h^2 k_z^2}{2 \mu} \right) \\
&\pm \frac{1}{2} \left( \frac{h^2 s^{-2}}{m_1} (n + 1/2) + \frac{h^2 k_z^2}{2 m_1} \right) \\
&\pm 4 \frac{h^2 s^{-2}}{m_2} (n + 1/2) + \frac{h^2 k_y^2}{2 m_2} + 4 |\Delta|^2/2.
\end{align*}$$

(78)

In the direction of perpendicular to the magnetic field

$$\begin{align*}
E_{n,\pm} &= \frac{1}{2} \frac{h^2 s^{-2}}{\mu} (n + 1/2) \\
&\pm \frac{1}{2} \sqrt{(\frac{h^2 s^{-2}}{\mu} (n + 1/2))^2 (\frac{1}{\mu^2} - \frac{4}{m_1 m_2}) + 4 |\Delta|^2},
\end{align*}$$

(79)

where $1/\mu = 1/m_1 + 1/m_2$, $m_1 = m^{(1)}$, $m_2 = m^{(2)}$.

Consider the limit analysis spectrum-wave vector dispersion for $\Delta \ll \hbar \omega_c$ and $\Delta \gg \hbar \omega_c$, where $\omega_c^{1,2} = \frac{h s^{-2}}{m_1, m_2}$. At
\[ \Delta \ll \hbar \omega_c \text{ and } |m_1 - m_2| > 0, \]

\[ E_{n,+} = (n + \frac{1}{2}) \frac{\hbar^2 s^{-2}}{m_1} + (n + \frac{1}{2}) \frac{\Delta^2}{\hbar^2 s^{-2} (m_1^{-1} - m_2^{-1})}, \]  
\( (80) \)

\[ E_{n,+} = (n + \frac{1}{2}) \frac{\hbar^2 s^{-2}}{m_2} - (n + \frac{1}{2}) \frac{\Delta^2}{\hbar^2 s^{-2} (m_1^{-1} - m_2^{-1})}. \]  
\( (81) \)

At \( \hbar \omega_c \ll \Delta \),

\[ E_{n,\pm} = \frac{1}{2} \hbar \omega_c^{\text{red}} (n + \frac{1}{2}) \pm |\Delta| \left( 1 + (n + \frac{1}{2})^2 \frac{\hbar^2 \omega_c^{(1)} \omega_c^{(2)}}{8 |\Delta|^2} \frac{(m_1-m_2)^2}{m_1 m_2} \right). \]  
\( (82) \)

If \( |m_1| = |m_2| \),

\[ E_{n,\pm} = \frac{1}{2} \hbar \omega_c^{\text{red}} (n + \frac{1}{2}) \pm |\Delta|. \]  
\( (83) \)

The envelope wave vector of quantized Landau levels:

\[ C_n^{(1)} = \left\| \frac{\frac{\delta}{2} - \tilde{\epsilon}_1 - \lambda_+}{\delta} \right\|, \]  
\( (84) \)

\[ C_n^{(2)} = \left\| \frac{\tilde{\epsilon}_1 - \lambda_+}{\frac{\delta}{2}} \right\|, \]  
\( (85) \)

where

\[ \delta = \sqrt{1 + (\tilde{\epsilon}_1 - \lambda_+)^2} = \sqrt{1 + (\tilde{\epsilon}_2 - \lambda_-)^2}, \]
\[ \tilde{\epsilon}_1 = \frac{\hbar^2 s^{-2}}{m_1 \Delta} (n + \frac{1}{2}), \]
\[ \tilde{\epsilon}_2 = \frac{\hbar^2 s^{-2}}{m_2 \Delta} (n + \frac{1}{2}), \]
\[ \lambda_+ = \frac{\epsilon_n \pm |\Delta|}{\delta}, \]  
\( (86) \)

\[ \epsilon_n = \frac{1}{2} \frac{\hbar^2 s^{-2}}{\mu} (n + \frac{1}{2}) + \frac{1}{2} \sqrt{\left( \frac{\hbar^2 s^{-2}}{\mu} (n + \frac{1}{2}) \right)^2 - \frac{4 |\Delta|^2}{m_1 m_2} + 4 |\Delta|^2}. \]

Wave vectors are built on Bloch vectors of z component of operator spin:

\[ \alpha = \left\| \frac{1}{0} \right\|, \]  
\( (87) \)

\[ \beta = \left\| 0 \frac{1}{1} \right\|. \]  
\( (88) \)

Indeed from (84) and (85) can build the unitary matrix, which acting on envelope wave vectors develops the basic wave vectors, which can be eigenwave vectors of z component of operator spin:

\[ \left\| \frac{1}{\delta} \frac{\tilde{\epsilon}_1 - \lambda_+}{\frac{\delta}{2}} \right\| = \left\| \frac{1}{0} \right\|, \]  
\( (89) \)
which corresponds eigenvalue $\hbar/2$,

$$
\left\| \frac{1}{3} \lambda \frac{\hat{\mathbf{r}}_1 - \lambda \hat{\mathbf{r}}_3}{\frac{1}{3}} \right\| \left\| \frac{\hat{\mathbf{r}}_1 - \lambda \hat{\mathbf{r}}_3}{\frac{1}{3}} \right\| \right\| 0 \right\|_1
$$

(90)

with eigenvalue $-\hbar/2$.

The Hamiltonian (64) describes two interacting harmonic oscillations with single common center or one-valley conduction band of virtual GaAsN crystal. Existing two solutions of dispersion equation leads to a duality conduction bandlike with high degree of non-parabolicity in selected gauge of vector potential in the perpendicular magnetic field in axes of effective mass tensor.

From dispersion dependence can to arrive to the conclusion that only such pairs of Landau levels of two harmonic oscillators are interacted: $1_+ \rightarrow 1_-, 2_+ \rightarrow 2_-, ..., $ that causes complex character of conduction band. Thus interaction character of Landau levels causes forming of complex one-valley band. Thus the conductor band has non-parabolic energy spectrum. The reducing of the band gap is due to the highly localized nature of the perturbation causes by substitution N atoms.

The largest contributions to the band gap reduction originate from structural relaxation and charge exchange that are, respectively, proportional to the differences in the atomic orbital size and energy of the As and N atoms in a simplest approach based on the virtual crystal approximation. This means that wavelength of spatial extension De-Broill wave function electrons is much larger than distance between neighbouring impurity N atoms. In this case the crystal with disordered and inhomogeneous solid solution can to change the random and homogeneous crystal. The accuracy estimation is equal of value of broadening with respect of split of two Landau levels.

Consider the energy of zero of Landau level in the plane of quantization which directs toward perpendicularly to highest symmetry point. From (92) can to draw a conclusion that

$$
\left\| \begin{array}{c}
\frac{1}{3} \lambda \\
\frac{1}{3} \lambda
\end{array} \right\| \left\| \begin{array}{c}
\frac{1}{3} \lambda \\
\frac{1}{3} \lambda
\end{array} \right\| = 0
$$

(95)

Thus from (95) can to arrive at a conclusion about the existing the symmetrical dependence of splitting $E_0^+$ and $E_0^-$ with respect to highest symmetry point. From (92) can to draw a conclusion that $\Delta_{1+} > \Delta_0^+, \Delta_{1-} > \Delta_1^-, ..., \Delta_{n+} > \Delta_n^-$ for 3-dimensional GaAsN in perpendicular magnetic field in axes of effective mass tensor $(m_{xx}^* m_{yy}^* m_{zz}^*)^{1/3}$. 

$$
E_{0}^\pm = \frac{\hbar^2 s^{-2}}{4m} \pm \sqrt{(\frac{\hbar^2 s^{-2}}{2})^2 (1 + \frac{1}{m_{1m_2}}) + 4|\Delta|^2}.
$$

(91)

The each next level is separated from antecedent on the value $E_{n+1}^\pm - E_{n}^\pm = \Delta_n^\pm$, where

$$
\Delta_n^\pm = \frac{\hbar^2 s^{-2}}{2m} \pm \sqrt{(\frac{\hbar^2 s^{-2}}{2})^2 (1 + \frac{1}{m_{1m_2}}) + 4|\Delta|^2}.
$$

(92)

Lowest energy level is defined as $n = 0$. In this case the energy oscillator is defined by (91). Thus for the harmonic oscillator the energy of zero level $E_0 = \frac{\hbar^2 s^{-2}}{2m}$. For the two harmonic oscillators the energy of zero salient level is equal

$$
E_{0}^+ = \frac{\hbar^2 s^{-2}}{4m} + \sqrt{(\frac{\hbar^2 s^{-2}}{2})^2 (1 + \frac{1}{m_{1m_2}}) + 4|\Delta|^2},
$$

(93)

while as for the concave energy level:

$$
E_{0}^- = \frac{\hbar^2 s^{-2}}{4m} - \sqrt{(\frac{\hbar^2 s^{-2}}{2})^2 (1 + \frac{1}{m_{1m_2}}) + 4|\Delta|^2}.
$$

(94)

Thus $E_{0}^+ = \epsilon + \lambda$, $E_{0}^- = \epsilon - \lambda$, where

$$
\epsilon = \frac{\hbar^2 s^{-2}}{4m},
$$

$$
\lambda = \sqrt{(\frac{\hbar^2 s^{-2}}{2})^2 (1 + \frac{1}{m_{1m_2}}) + 4|\Delta|^2}.
$$

(95)
Researching the found expression (92) can to reach a conclusion that

\[ \Delta_0 > \Delta_1 > \Delta_2 > \ldots > \Delta_{-1} > \Delta_{-k} > \ldots \]  \hspace{1cm} (96)

Thus series \( \Delta_0, \Delta_1, \Delta_2, \ldots, \Delta_{-1}, \Delta_{-k}, \ldots \) are convergent as well as can lead to transformation discrete spectrum into continuous one that is into compression levels. That is the possibility of existing of bound state at consideration of two harmonic oscillators with single center in 1-dimensional space is shown.

In the article the conduction bands of dilute GaAsN, in the case when \( n^{(2)} \to \infty \) are studied. For 0.1% N with 0.2 eV localized N-impurity level with respect of edge conduction band and hybridization between extended states of semiconductor matrix and orbits of N atoms occurs at \( k = 6 \times 10^8 \text{m}^{-1} \) calculated from Brillouin zone center, need to apply of magnetic field of 15.4 T, in order to tune an electron into a given \( k \) state. Thus it is shown, that the formalism can be used in the magnetotunneling spectroscopy researches.

D. Results and their discussions

Numerically solving the microscopic polarization equations for the quantum well with parabolic band, one can see that with increasing an electron-hole gas density optical gain develops in the spectral region of the original exciton resonance. With increasing the free-carrier density the ionization continuum red shifts rapidly to long wavelength, while the 1s-exciton absorption line stays almost constant, due to the high degree of compensation between the weakening of the electron-hole binding energy and band-gap reduction. Physically it indicates the charge neutrality of an exciton. The calculated Hartree-Fock spectra for the exciton in the wurtzite quantum well with parabolic bands are shown in Fig. 1. All calculations are carried at the temperature 300 K.

In the paper the energy of the exciton resonance are shown to be calculated at 3749.5 meV for a concentration of carriers \( 5 \times 10^{11} \text{ cm}^{-2} \).

Unlike will be develop the process of shifting of the absorption edge at the constant of exciton energy with increasing concentrations for wurtzite quantum well. Solving the polarization equation in Hartree-Fock approximation one can find red shifting of exciton resonance with increasing concentration in the wurtzite quantum well. The calculated Hartree-Fock spectra for the exciton in the wurtzite quantum well of width of 2 nm is presented in Fig. 2.

Such shifting may be explained of the difference between the overlap integrals of the electron and hole wave functions both the wurtzite quantum well and quantum well with parabolic band. The overlap integral of the electron and hole wave functions at nonzero wave vectors in the wurtzite quantum well has smaller value than the overlap integral in the quantum well with parabolic band. Due to this cause the Coulomb renormalization of the electric dipole moment in (57) in the wurtzite quantum well is found to be smaller than in quantum well with the parabolic band and will can not compensate Coulomb renormalization of the self energy in (56), which is included in equation (55) with minus sign. This implies the shifting of the exciton resonance in the side of the less energy. Since shifts in the exciton resonance are very rare effect, examples of exceptions are always interesting.

Hartree and Hartree-Fock gain spectra are presented in Fig. 3.

The energy spectrum for heavy, light holes for the quantum well is presented in Fig. 4, and also Hartree and Hartree-Fock renormalization of the energy spectrum for heavy, light holes and electrons which reflect many-body effect known as renormalization band gap were calculated.

Electron and photon teleportation in quantum spectroscopy researches are shown to be related with a significant shift of the exciton peak in materials with complex dispersion. The entanglements of doubled conduction band one can lead into electron teleportation, quantum cryptography and artificial intelligence researches.

E. Summary

The calculations of a light gain spectrum and exciton spectrum previously where carried only for the nitride quantum well with parabolic bands and where not carried for the quantum well with compound band. In the paper we presented the study of nonparabolicity on exciton state in wurtzite quantum well. We have calculated and have explained that caused by dependency the exciton binding energy from overlap integral of the electron and hole wave functions the exciton binding energy strongly depends from exist valence bands mixing. Laser technology has revolutionized the study of nonparabolicity on exciton state in wurtzite quantum well. We have calculated and have explained shifting of the exciton resonances which depend from an electron-hole gas concentration. We calculated the ship of gain spectrum in the wurtzite quantum well. We calculated the exchange renormalization of the energy spectrum for a holes and
electrons. In the research of the influence of the overlap integral of wave functions on Hartree-Fock renormalization of the electric dipole moment in the wurtzite quantum well can derive the following summary: the deviate from parabolic band structure in wurtzite quantum well leads to significant changes in the determination of the exciton binding energy. The calculations testify about the small change of the overlap integral of the electron and hole wave function which is caused the intrinsic quantum confined Stark effect at the considered concentrations of an electron-hole gas. The deviate from the parabolic band structure of the quantum well leads to significant changes in overlap integral of the electron and hole wave functions. This is of cause of the red shift of exciton resonance with increasing concentrations of an electron-hole gas. The calculated results can be explained by an influence of the valence band structure on quantum confined effects.

II. LOCAL EXCHANGE-CORRELATIONAL POTENTIAL ON PARTICLE-HOLE PAIRING IN SUPERCONDUCTING STATE IN ZNO/(ZN,MG)O QUANTUM WELLS

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 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 addition. The shifts of the Hartree valence band spectrums and the conduction band spectrum with respect to the flat band spectrums as well as the Hartree-Fock band spectrums with respect to the Hartree one are found. An overlap integrals of the wave functions of holes and electron with taking into account besides the piezoelectric effects the exchange-correlation effects in addition is greater than an overlap integral of Hartree ones. The Hartree particles distribute greater on edges of quantum well than Hartree-Fock particles. It is found that an effective mass of heavy hole of Mg$_{0.27}$Zn$_{0.73}$O under biaxial strain is greater than an effective-mass of heavy hole of ZnO. It is calculated that an electron mass is less than a hole mass. It is found that the Bohr radius is greater than the localization range particle-hole pair, hence the excitons may be spontaneously created.

There has been widely studied in the ultraviolet spectral range lasers based on direct wide-bandgap hexagonal wurtzite crystal material systems such as ZnO$^{74-79}$. Significant success has been obtained in growth ZnO quantum wells with (ZnMg)O barriers by scrutinized methods of growth$^{80,81}$. The carrier relaxation from (ZnMg)O barrier layers into a ZnO quantum well through time-resolved photoluminescence spectroscopy is studied in the paper$^{82}$. The time of filling of particles for the single ZnO quantum well is found to be 3 ps$^{82}$.

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$^{83}$, 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$^{84,85}$. 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$^8$ including deformation potentials$^{86}$. 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.

In this paper we present a self-consistent calculation an above mentioned equations in wurtzite ZnO quantum well taking into account the piezoelectric effect and the exchange-correlation potential for bandgap renormalization and engineering of localized Hartree-Fock wave functions. The energy shifts as well as the localization range of exchange-correlational wave functions with respect to Hartree energy shifts and Hartree localization range of wave functions require a scrutiny study.

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 superconductivity. If the exciton binding energy is grater than the localization range particle-hole pair, the excitons may be spontaneously created.
A. Theoretical study

1. Effective Hamiltonian

It is known\(^6,69\) that the valence-band spectrum of hexagonal würtzite crystal at the \(\Gamma\) point originates from the sixfold degenerate \(\Gamma_{15}\) state. Under the action of the hexagonal crystal field in würtzite crystals, \(\Gamma_{15}\) splits and leads to the formation of two levels: \(\Gamma_1, \Gamma_5\). The wave functions of the valence band transform according to the representation \(\Gamma_1 + \Gamma_5\) of the point group \(C_{6v}\), while the wave function of the conduction band transforms according to the representation \(\Gamma_1\).

<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>(\Gamma_1 + \Gamma_5)</td>
<td>3</td>
<td>-1</td>
<td>0</td>
<td>2</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>(g^2)</td>
<td>(E)</td>
<td>(E)</td>
<td>(C_3)</td>
<td>(C_3)</td>
<td>(E)</td>
<td>(E)</td>
</tr>
<tr>
<td>(\chi_v^2(g))</td>
<td>9</td>
<td>1</td>
<td>0</td>
<td>4</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>(\chi_v(g^2))</td>
<td>3</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>(\frac{1}{2} [\chi_v^2(g) + \chi_v(g^2)])</td>
<td>6</td>
<td>2</td>
<td>0</td>
<td>2</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>(\frac{1}{2} [\chi_v^2(g) - \chi_v(g^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 presentations for orbital angular momentum \(j\) may be built from formula

\[
\chi_j(\varphi) = \frac{\sin (j + \frac{1}{2}) \varphi}{\sin \frac{\varphi}{2}}.
\]

(97)

For the vector representational \(j = 1\)

\[
\chi_v(\varphi) = \frac{\sin 3\varphi}{\sin \frac{3\varphi}{2}} = 1 + 2 \cos \varphi.
\]

(98)

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

\[
p^{\alpha} : \tau_v \times \tau_\psi = (\Gamma_1 + \Gamma_5) \times (\Gamma_2 + \Gamma_5) = \Gamma_5 \times \Gamma_5,
\]

(99)

for the square of wave vector

\[
[p^{\alpha}p^\beta] : \tau_{v\alpha} \times \tau_\psi = (2\Gamma_1 + \Gamma_5 + \Gamma_6) \times (2\Gamma_1 + \Gamma_5 + \Gamma_6) = 4\Gamma_1 \times \Gamma_1 + \Gamma_5 \times \Gamma_5 + \Gamma_6 \times \Gamma_6.
\]

(100)

In the low-energy limit the Hamiltonian of würtzite

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

(101)

\[
\hat{H}_k = A_1 k_x^2 + A_2 k_y^2 + (A_3 k_x^2 + A_4 k_y^2) J_z^2 + \\
+ A_5 k_z (2[J_+ J_-] k_- + 2[J_z J_-] k_z) + \\
+ A_6 (J_+ k_-^2 + J_- k_+^2) + i A_7 (J_+ k_- - J_- k_+),
\]

(102)
\[ \hat{H} = D_1 \varepsilon_{zz} + D_2 \varepsilon_{zz}^2 + (D_3 \varepsilon_{zz} + D_4 \varepsilon_\perp) J_z^2 + \\
+ D_5 (2|J_z J_+| \varepsilon_{zz} + 2|J_z J_-| \varepsilon_{zz} + 2|J_z J_+| \varepsilon_{zz} + 2|J_z J_-| \varepsilon_{zz}) + \\
+ D_6 (J_z^2 \varepsilon_\perp + J_z^2 \varepsilon_\perp). \quad (103) \]

In the basis of spherical wave functions with the orbital angular momentum \( l = 1 \) and the eigenvalue \( m_l \) of its \( z \) component:

\[
\begin{align*}
|1, s_\nu\rangle &= \frac{1}{\sqrt{2}} \left( Y_1^1 \psi(1/2)e^{-3i\varphi/2}e^{-i\varphi/4} \pm Y_1^{-1} \psi(-1/2)e^{3i\varphi/2}e^{i\varphi/4} \right) \\
|2, s_\nu\rangle &= \frac{1}{\sqrt{2}} \left( \pm Y_1^1 \psi(-1/2)e^{-i\varphi/2}e^{-i\varphi/4} + Y_1^{-1} \psi(1/2)e^{i\varphi/2}e^{i\varphi/4} \right), \\
|3, s_\nu\rangle &= \frac{1}{\sqrt{2}} \left( Y_0^0 \psi(1/2)e^{-i\varphi/2}e^{-i\varphi/4} + Y_0^0 \psi(-1/2)e^{i\varphi/2}e^{i\varphi/4} \right).
\end{align*}
\quad (104)
\]

the Hamiltonian may be transformed to the diagonal form indicating two spin degeneracy \( ^s \) :

\[
H_\pm = \begin{pmatrix}
F & K_t \\
K_t & G
\end{pmatrix} \pm iH_t = \begin{pmatrix}
|1, s_\nu\rangle \\
±i|H_t| |3, s_\nu\rangle
\end{pmatrix}, \quad (105)
\]

where \( F = D_1 + D_2 + \lambda + \theta, G = D_1 - D_2 + \lambda + \theta, \lambda = \lambda_k + \lambda, \theta = \theta_k + \theta, \lambda_k = \frac{\hbar^2}{2m_\nu} (A_k k_z^2 + A_k k_z^2), \lambda = D_1 \varepsilon_{zz} + D_2 (\varepsilon_{xx} + \varepsilon_{yy}), \theta_k = \frac{\hbar^2}{2m_\nu} (A_3 k_z^2 + A_3 k_z^2), \theta = D_3 \varepsilon_{zz} + D_4 (\varepsilon_{xx} + \varepsilon_{yy}), K_t = \frac{\hbar^2}{2m_\nu} (A_6 k_z^2), H_t = \frac{\hbar^2}{2m_\nu} (A_6 k_z^2), \Delta = \sqrt{2} \Delta_3, k_z^2 = k_3^2 + k_0^2.
\]

From Kane model one can define the band-edge parameters such as the crystal-field splitting energy \( \Delta_{cr} \), the spin-orbit splitting energy \( \Delta_{so} \) and the momentum-matrix elements for the longitudinal (\( x \mid z \)) \( z \)-polarization: \( P_x \equiv \langle S|\hat{p}_x|Z \rangle, P_\perp = \langle S|\hat{p}_x|X \rangle \equiv \langle S|\hat{p}_y|Y \rangle \). Here we use the effective-mass parameters, energy splitting parameters, deformation potential parameters as in papers\(^{10,86,88}\).

We consider a quantum well of width \( w \) in ZnO under biaxial strain, which is oriented perpendicularly to the growth direction \((001)\) 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 \( x \) : \( \varepsilon_{xx} = \varepsilon_{yy} = \frac{a_{ZnO} - a_{ZnO}}{a_{ZnO} - a_{MgO}}, a_{ZnO} = 0.32946, a_{MgO} = 0.4216, 10 \). The longitudinal component of a deformation is expressed through elastic constants and the transverse component of a deformation: \( \varepsilon_{zz} = \frac{2C_{33}}{E_{33}} \varepsilon_{xx} \).

The physical parameters for ZnO are as follows. We take the effective-mass parameters \( ^8 \) : \( A_1 = -2.743, A_2 = -0.393, A_3 = 2.377, A_4 = -2.069, A_5 = -2.051, A_6 = -2.099, m_e^{3/2} = 0.32946, m_h \) is the electron rest mass in the vacuum, the parameters for deformation potential \( ^8 \) : \( D_1 = -3.800 \text{ meV}, D_2 = -3.800 \text{ meV}, D_3 = -800 \text{ meV}, D_4 = 1400 \text{ meV}, D_\perp = -8600 \text{ meV}, D_\parallel = -6260 \text{ meV}, \) and the energy parameters at \( 300 \text{ K} \). \( E_g = 3.400 \text{ meV}, \Delta_1 = \Delta_{so} = 63.3 \text{ meV}, \Delta_2/3 = 0.63 \text{ meV}, \Delta_3/3 = 2.47 \text{ meV}, \Delta_2 = \Delta_3 = \Delta_{so} \) the elastic constant \( ^{10} \) : \( C_{13} = 90 \text{ GPa} \) and \( C_{33} = 196 \text{ GPa} \), the permittivity of the host materials \( \kappa = 7.8. \)

2. ZnO/(Zn,Mg)O quantum well

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

\[
|\nu, s_\nu, k_z\rangle = \sum_{m=0}^{m} |\Psi_\nu^{(1)}[i, \nu] \psi_i(Z)| |1, s_\nu\rangle \\
+ \sum_{m=0}^{m} |\Psi_\nu^{(2)}[i, \nu] \psi_i(Z)| |2, s_\nu\rangle \\
+ \sum_{m=0}^{m} |\Psi_\nu^{(3)}[i, \nu] \psi_i(Z)| |3, s_\nu\rangle \quad (106)
\]

The Bloch vector of \( \nu \)-type hole with spin \( s_\nu = \pm 1/2 \) and momentum \( k_z \) is specified by its three coordinates \( [\Psi_\nu^{(1)}[m, \nu], \Psi_\nu^{(2)}[m, \nu], \Psi_\nu^{(3)}[m, \nu]] \) in the basis \( |[1, s_\nu\rangle, [2, s_\nu\rangle, [3, s_\nu\rangle] \) \( ^8 \), known as spherical harmonics with the orbital angular
momentum \( l = 1 \) and the eigenvalue \( m_l \) 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

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

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

\[
\Psi_{\nu, k_z}(r) = \frac{e^{ik_z \rho_m}}{\sqrt{\lambda}} |\nu, k_z\rangle.
\]

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

\[
\sum_{j=1}^{3}(H_{ij}^{(v)}(k_z) = -i \frac{\partial}{\partial z} + V(z) + \delta_j E_{\nu}^{(v)}(k_t)) \times \phi_{\nu}^{(v)}(z, k_t) = 0,
\]

where \( \phi_{\nu}^{(v)}(z, k_t) = \sum_{n=1}^{m} \Psi_{k_t}^{(v)}[n, \nu] \psi_n(z), \ i = 1, 2, 3. \)

The wave function of electron of first energy level with accounts QCSE \( 89 \):

\[
\Psi(r) = \frac{1}{\sqrt{A}} e^{ik_z \rho_m} \psi(Z, \xi)|S| |\xi_c\rangle,
\]

where

\[
\psi(Z, \xi) = \begin{cases} 
\psi_1(Z, \xi) = C_1 e^{(ka - \xi w)(w Z)}, Z \in (-\infty, 0) \\
\psi_2(Z, \xi) = C \sin((k_0 w (Z - \frac{1}{2}) + \delta_0)e^{-\xi w (Z - \frac{1}{2})}, Z \in [0, 1] \\
\psi_3(Z, \xi) = C_2 e^{-(ka - \xi w)(w Z)}, Z \in (1, \infty). 
\end{cases}
\]

| \( S \) = \( Y_0 \), \( \xi_c = \pm 1/2 \).

From bond conditions \( 36, 89 \), \( \psi_1(Z, \xi)|_{Z=0} = \psi(Z, \xi)|_{Z=0}, \psi_2(Z, \xi)|_{Z=1} = \psi(Z, \xi)|_{Z=1}, \frac{\psi_1(Z, \xi)}{\psi_3(Z, \xi)}|_{Z=0} = \frac{\psi_3(Z, \xi)}{\psi_1(Z, \xi)}|_{Z=0}, \psi_1(Z, \xi)|_{Z=1} = \psi_2(Z, \xi)|_{Z=1}, \) one can find \( C_1 = C \sin(-k_0 w + \delta_0)e^{\xi\pi}, C_2 = C \sin(\frac{k_0 w}{2} + \delta_0)e^{-\xi\pi}, \kappa_0 = k_0(1 - \cos k_0 w), \delta_0 = \frac{k_0 w}{2} + \arctan \frac{2w}{k_0}, \) where \( A \) is the area of the quantum well in the \( xy \) plane, \( \rho \) is the two-dimensional vector in the \( xy \) plane, \( k_t = (k_x, k_y) \) is in-plane wave vector. The constant multiplier \( C \) is found from normalization condition:

\[
\int_{-\infty}^{\infty} |\psi(Z, \xi)|^2 w dZ = 1. \]
Figure 9. (Color online) For the quantum well ZnO/Mg0.27Zn0.73O with a width 4 nm, at a carriers concentration \(4 \times 10^{12} \text{ cm}^{-2}\), at a temperature 300 K: (a) Hartree screening potential; (b) Hartree-Fock screening potential.

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

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

(113)

where

\[
\hat{H} = H_c + V(z),
\]

(114)

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

\[
H_c = E_g + \Delta_1 + \Delta_2 + \frac{\hbar^2}{2m_e} k^2 - \frac{\hbar^2}{2m_e} \nabla^2 + D_{zz} \epsilon_{zz} + D_{\perp}(\epsilon_{xx} + \epsilon_{yy}).
\]

(115)

The potential energies \(V(z)\) can look for as follows:

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

(116)

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 bandedge discontinuities which can be represented in the form \(90\):

\[
\delta U_c(z) = \begin{cases} 
U_0 - eEw(\frac{z}{w} + 1), z \in (-\infty, -w/2) \\
U_0 - eEw(\frac{z}{w} - 1), z \in (w/2, \infty).
\end{cases}
\]

(117)

\(\Phi_{xc}(z)\) is exchange-correlation potential energy which is found from the solution of three-dimensional Poisson’s equation, using both an expression by Gunnarsson and Lundquist \(91\), and following criterions. At carrier densities \(4 \times 10^{12} \text{ cm}^{-2}\), the criterion \(k_F > \sqrt{n}/4\) at a temperature \(T=0\) K as \(1 > 0.1\) has been carried. \(k_F\) is Fermi wave vector. The criterion does not depend from a width of well. The ratio of Coulomb potential energy to the Fermi energy is \(r_s = E_C/E_F \approx 0.63 < 1\). 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 using a criterion \(|\Psi_{\alpha,v,n}(k_F, z) \sin k_F \rho| << 1\), where \(\alpha = e, h\).

The three-dimensional Poisson’s equation includes local exchange-correlation potential:

\[
\frac{d^2 \Phi_{e,h}}{dz^2} + \Delta_p \Phi_{e,h} = \frac{4\pi}{\kappa} \rho_{e,h}(z; g) + \rho^{xc}_{e,h}(r, r'),
\]

(118)

\[
\frac{d^2 \Phi_{e,h}}{dz^2} = \frac{4\pi}{\kappa} \rho_{e,h}(z; g),
\]

(119)
\[ \Delta \phi \Phi_{e,h}^{xc} = \frac{4\pi}{\kappa} \rho_{e,h}^{xc}(r,r'), \]  

(120)

where

\[ \rho_{e,h}^{H}(z; g) = \mp e \sum_{\nu,n,k_i} |\Psi_{e,h,v,n}(k_i; z)|^2 f_{n,v}(k_i; g), \]

(121)

\[ f_{n,v}(k_i; g) = \frac{1}{e^{(\nu,n,k_i + \frac{2}{3} + \sum j \frac{1}{\gamma_j})} + 1} = \frac{1}{e^{(1 + \nu, + n, + \frac{2}{3} + \sum j \frac{1}{\gamma_j})} + 1}. \]

(122)

The solution of equations system (109), (113), (118) as well as (109), (113), (119) does not depend on the temperature.

Solving one-dimensional Poisson’s equation (119) one can find screening polarization field and Hartree potential energy by substituting her in the Schrödinger equations. From Schrödinger equations wave functions and band structure are found. The conclusive determination of screening polarization field is determined by iterating Eqs. (109), (113), (118) until the solutions of conduction and valence band energies and wave functions are converged:

\[ \Phi_{H}^{H}(z) = \Phi_{e}^{H}(z) + \Phi_{e}^{H}(z), \]

(123)

\[ e\Phi_{h}^{H}(z) = \frac{2\zeta^2}{\kappa} \sum_{\nu,m,l,i} g_1 \int k_i dk_i \langle v_i, s_i | \Psi_{h,k_i} | \nu', m' | | \nu, v_i \rangle f_{\nu,p}(k_i) \times \]

\[ w_{\nu}(\cos \pi(\frac{1}{2}(l+m)) - \cos \pi(\frac{1}{2}(m-l))), m \neq l \]

\[ w_{\nu}(\frac{\Phi_{h,0}}{2} + \frac{1}{2} \cos \pi\nu\frac{1}{2}(\frac{1}{2} + \frac{3}{2})), m = l \]

(124)

\[ e\Phi_{h}^{H}(z) = -\frac{2\zeta^2}{\kappa} \int k_i dk_i C_{\nu} f_{1n}(k_i) \times \]

\[ \frac{1 - \cos(-k_0 w + 2h_0)}{\sqrt{4(\zeta^2 + k_0^2)}} e^{-\zeta z} - \frac{2}{\zeta}\frac{2 \cos(2k_0 w + 4h_0)}{4(\zeta^2 + k_0^2)} \frac{e^{-\zeta z}}{\sin(2k_0 + \frac{\gamma}{2}) - e^{-\zeta z}} k_0 \xi, z \in [-w/2, w/2] \]

\[ \frac{1 - \cos(-k_0 w + 2h_0)}{\sqrt{4(\zeta^2 + k_0^2)}} e^{-\zeta z} + \frac{2}{\zeta}\frac{2 \cos(2k_0 w + 4h_0)}{4(\zeta^2 + k_0^2)} \frac{e^{-\zeta z}}{\sin(2k_0 + \frac{\gamma}{2}) - e^{-\zeta z}} k_0 \xi, z \in (w/2, \infty), \]

(125)

where \( Z = \frac{\zeta}{2} + \frac{1}{2}, g_1 \) and \( g_1 \) correspond to the degeneracy of the \( \nu \) hole band and the first quantized conduction band, \( e \) is the value of electron charge, \( \kappa \) is the permittivity of a host material, and \( f_{\nu,p}(k_i), f_{1n}(k_i) \) are the Fermi-Dirac distributions for holes and electrons.

Exchange-correlation charge density may be determined as:

\[ \rho_{e,h}^{xc}(r,r') = \sum_{l,m=-l}^{l} |\Psi_{\alpha,v,n}(k_i, z)|^2 \rho_{lm}(r - r') Y_{lm}(\frac{r - r'}{r - r'}), \]

(126)

using the expansion of plane wave

\[ \sum_{l=0}^{l} \sum_{m=-l}^{l} \rho_{lm}(r) Y_{lm}(\frac{r}{r}) = \]

\[ e^{i k_i \rho} = 4\pi \sum_{l=0}^{l} \sum_{m=-l}^{l} \frac{i l}{r} j_l(k_i, r) Y_{lm}(\frac{k_i}{r}) Y_{lm}(\frac{r}{r}). \]

(127)

At the condition \( |\Psi_{\alpha,v,n}(k_F, z) \sin k_F r| << 1 \), the solution Eq. (120) may be found as follows

\[ \Phi_{e,h}(xe) = \int_0^\infty \rho r_0(\rho) \frac{1}{r_0} d\rho. \]

(128)

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

\[ \Phi_{e,h}(z) = \Phi_{e,h}(z) \Phi_{e,h}(xc). \]

(129)

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

$$\Phi(z) = \Phi^H_H(z) + \Phi^H_e(z) + \Phi^H_e(z) \Phi^H_h(xc) + \Phi^H_e(z) \Phi_e(xc).$$  (130)

3. Uncertainty Heisenberg principle

The Heisenberg equation for a microscopic dipole $\hat{p}_{\nu e}^{\nu h}$ due to an electron-hole pair with the electron (hole) momentum $\mathbf{p}$ ($-\mathbf{p}$) and the subband number $\nu_e$ ($\nu_h$) is written in the form:

$$\frac{\partial \hat{p}_{\nu e}^{\nu h}}{\partial t} = \frac{i}{\hbar} [\hat{\mathcal{H}}, \hat{p}_{\nu e}^{\nu h}].$$  (131)

We assume a nondegenerate situation described by the Hamiltonian $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{V}} + \hat{\mathcal{H}}_{\text{int}}$, which is composed of the kinetic energy of an electron $\epsilon_{\nu e}^{\nu e}$ and the kinetic energy of a hole $\epsilon_{\nu h}^{\nu h}$ in the electron-hole representation:

$$\hat{\mathcal{H}}_0 = \sum_{\mathbf{p}} \epsilon_{\nu e}^{\nu e} \mathbf{a}^+_p \mathbf{a}_p + \epsilon_{\nu h}^{\nu h} \mathbf{b}^+_p \mathbf{b}_p + \mathbf{a}^+_p \mathbf{b}_p + \mathbf{b}^+_p \mathbf{a}_p,$$  (132)

where $\mathbf{p}$ is the transversal quasimomentum of carriers in the plane of the quantum well, $\mathbf{a}_p$, $\mathbf{a}^+_p$, $\mathbf{b}_p$, and $\mathbf{b}^+_p$ 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:

$$\hat{\mathcal{V}} = \frac{1}{2} \sum_{\mathbf{p,k},q} V^{\nu e}_{\nu h} V^{\nu h}_{\nu e} \mathbf{a}^+_p \mathbf{a}^+_q \mathbf{a}^-_{k-q} \mathbf{b}^+_k \mathbf{b}^-_p +$$

$$+ V^{\nu h}_{\nu e} V^{\nu e}_{\nu h} \mathbf{b}^+_p \mathbf{b}^+_q \mathbf{b}^-_{k-q} \mathbf{a}^+_k \mathbf{a}^-_p -$$

$$- 2 V^{\nu e}_{\nu h} V^{\nu h}_{\nu e} \mathbf{a}^+_p \mathbf{a}^+_q \mathbf{b}^+_k \mathbf{b}^-_p,$$  (133)

where

$$V^{\nu e}_{\nu h} V^{\nu h}_{\nu e} = \frac{e^2}{\kappa} \int_{-w/2}^{+w/2} dz \int_{-w/2}^{+w/2} dz' \chi_{\nu e}(z) \chi_{\nu h}(z') \frac{2\pi}{q} x.$$
The transverse effective masses for Al$_{0.3}$Ga$_{0.7}$N under biaxial strain: (a) for the heavy hole; (b) for the light hole.

\[ \times e^{-q|z-z'|} \chi_{\nu_h}(z') \chi_{\nu_h}(z), \]

is the Coulomb potential of the quantum well, $\kappa$ 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:

\[ \hat{H}_{\text{int}} = -\frac{1}{A} \sum_{\nu_e, \nu_h} ((\mu_{p\nu_e\nu_h})^* \hat{p}_{\nu_e\nu_h} E^* e^{i\omega t} + \text{c.c.}) + (\mu_{p\nu_e\nu_h}) (\hat{p}_{\nu_e\nu_h})^* E e^{-i\omega t}), \]

where $\hat{p}_{\nu_e\nu_h}=(\hat{b}_{-\nu_h} \hat{a}_{\nu_e})$ is a microscopic dipole due to an electron-hole pair with the electron (hole) momentum $p (-p)$ and the subband number $\nu_e (\nu_h)$. $\mu_{k\nu_e\nu_h} = \int d^3x U_{j'\sigma'k} e \sigma \nu e, p \nu h, k$ 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 $U_{j'\sigma'k}, U_{j\sigma k}$, where $j'$ is the number of a subband from the conduction band, $\sigma'$ 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\textsuperscript{85,92}, 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:

\[ \frac{d\hat{p}_{\nu_e\nu_h}}{dt} = -\hat{\omega}_{p\nu_e\nu_h} \hat{p}_{p\nu_e\nu_h} - i \Omega_{p\nu_e\nu_h} (-1 + \hat{n}_{p\nu_e} + \hat{n}_{p\nu_h}), \]

The transition frequency $\omega_{p\nu_e\nu_h}$ and the Rabi frequency with regard for the wave function\textsuperscript{85,92} are described as

\[ \omega_{p\nu_e\nu_h} = \frac{1}{\hbar} (\epsilon_{0\nu_e} + \epsilon_{p\nu_e} + \epsilon_{p\nu_h}), \]

\[ \Omega_{p\nu_e\nu_h} = \frac{1}{\hbar} (\mu_{p\nu_e\nu_h} E e^{-i\omega t} + \sum_{q} \left\{ \frac{1}{|q|} \right\} V_{p\nu_e\nu_h, p\nu_h} \hat{p}_{q\nu_e\nu_h}), \]

where $\epsilon_{p\nu_e}, \epsilon_{p\nu_h} -$ Hartree–Fock energies for electron and holes.
Figure 12. (Color online) For the quantum well ZnO/Mg$_{0.27}$Zn$_{0.73}$O with a width 4 nm, at a carriers concentration $4 \times 10^{12}$ cm$^{-2}$, at a temperature 300 K, at a transverse wave vector $k_t = 2 \times 10^7$ cm$^{-1}$: (a) Square of Hartree wave functions; (b) Square of Hartree-Fock wave functions.

$V^{\nu_e,\nu_h,\nu_e}_{\nu_e,\nu_h,\nu_e} = \frac{1}{2} \frac{e^2}{\kappa} \sum_{\alpha} g_{\alpha} \int dq \times$

$\times \int dz_\xi \int dz_{\xi'} \chi_{n_1}(z_\xi)\chi_{m_1}(z_{\xi'})\chi_{m_2}(z_{\xi'})\chi_{n_2}(z_\xi) \times$

$\times e^{-q|z_\xi-z_{\xi'}|} C_p^{[n_1,1]} V_p^{[m_1,1]} C_{Q_1}^{[n_2,1]} V_{Q_1}^{[m_2,1]}$

$n_1 = m_1 = n_2 = m_2 = 1,$

$Q_1 = q + p,$

(139)

where $\chi_{n_i}(z_\xi)$ is the envelope of the wave functions of the quantum well, $V_p^{[m_1,1]}$ and $C_p^{[n_1,1]}$ 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:

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

(140)

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

$P = \frac{2}{A} \sum_{\nu_e,\nu_h,p} (\mu_{\nu_e,\nu_h}^p)^* \nu_e,\nu_h e^{i\omega t}.$

(141)

The light absorption spectrum presented in the paper in Fig. 14, reflects only the strict TE ($x$ or $y$) light polarization. From Uncertainty Heisenberg principle:

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

(142)

can be found the localization range particle-hole pair $\Delta x \geq \frac{\hbar}{4mc}$. 
Fig. 13. (Color online) For the quantum well ZnO/Mg$_{50.27}$Zn$_{0.73}$O with a width 4 nm, at a carriers concentration $4 \times 10^{12}$ cm$^{-2}$, at a temperature 300 K: (a) Hartree charge density; (b) Hartree-Fock charge density.

Table 1. The localization range particle-hole pair $\Delta x$ in cm, exciton binding energy $R_y$ in meV, carriers concentration $n = p$ in cm$^{-2}$, Bohr radius $a_B$ in cm.

<table>
<thead>
<tr>
<th>$\Delta x$</th>
<th>$R_y$</th>
<th>$n-p$</th>
<th>$a_B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$5.58 \times 10^{-11}$</td>
<td>38.53</td>
<td>$4 \times 10^{12}$</td>
<td>$2.39 \times 10^{-7}$</td>
</tr>
</tbody>
</table>

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

4. Results and discussions

We consider QCSE in strained wurtzite ZnO/Mg$_{50.27}$Zn$_{0.73}$O quantum well with width 4 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. All calculations are performed at a temperature of 300 K.

We have calculated carriers population of the lowest conduction band and the both heavy hole and light hole valence band. Solving (109) for holes in the infinitely deep quantum well and finding the minimum of functional (113) 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. (109), (113), (118) until the solution of energy spectrum is converged.

The dispersion of the renormalization band gap is presented in Fig. 8. We have found $E_g^{HF} - E_g^{Flatband} = 20.72$ meV, $E_g^{HF} - E_g^{H} = 4.40$ meV, comparing the Hartree band gap with the flat band gap as well as the Hartree-Fock band gap. Comparing $E_g^{HF}$ and $E_g^{H}$ and a shape of bedplate of quantum well for electrons which is presented in Fig. 9 as well as a same shape of bedplate of quantum well for holes one can see that an electron mass is less than a hole mass. The effective masses Mg$_{50.27}$Zn$_{0.73}$O under biaxial strain for the heavy holes and light holes are presented in Fig. 10. Both the effective mass of Mg$_{50.27}$Zn$_{0.73}$O under biaxial strain for the heavy hole and the effective mass of Al$_{0.3}$Ga$_{0.7}$N under biaxial strain for the heavy hole are presented in Fig. 11. From these Figures one can see that a mass of heavy hole of Mg$_{50.27}$Zn$_{0.73}$O is greater than a mass of heavy hole of Al$_{0.3}$Ga$_{0.7}$N. Comparing the effective mass of Mg$_{50.27}$Zn$_{0.73}$O under biaxial strain for the heavy hole with an effective-mass parameter $A_1 = -2.743$ one can conclude that an effective mass of heavy hole of Mg$_{50.27}$Zn$_{0.73}$O under biaxial strain is greater than an effective-mass of heavy hole of ZnO.

The squares of Hartree and Hartree-Fock wave functions for electrons, heavy holes and light holes are presented in Fig. 12. From Fig. 12 one can conclude that an overlap integrals of the wave functions of holes and electron taking into the account besides the piezoelectric effects the exchange-correlation effects in addition are greater than
an overlap integrals of Hartree ones. Hartree charge density distribution and Hartree-Fock charge density distribution are presented in Fig. 13. Comparing charge density distributions presented in Fig. 13 one can conclude that Hartree particles distribute greater on edges of quantum well than Hartree-Fock particles. It is found that the localization range particle-hole pair $\Delta x \geq \frac{h}{mc_0} \sim 5.58 \times 10^{-11}$ cm. Exciton binding energy is equal $\text{Ry}=38.53$ meV at carriers concentration $n = p = 4 \times 10^{12}$ cm$^{-2}$. Bohr radius is equal $a_B = 2.39 \times 10^{-7}$ cm.

If the Bohr radius is greater than the localization range particle-hole pair, the excitons may be spontaneously created.

### B. Appendix I

<table>
<thead>
<tr>
<th>$C_{6\nu}$</th>
<th>$E$</th>
<th>$C_2$</th>
<th>$2C_3$</th>
<th>$2C_8$</th>
<th>$3\sigma_v$</th>
<th>$3\sigma'_v$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Gamma_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>$k_z^2, k_l^2, J_z^2, I$</td>
</tr>
<tr>
<td>$\Gamma_2$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>$J_z, \sigma_z$</td>
</tr>
<tr>
<td>$\Gamma_3$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>$J_+, \sigma_+, J_-, \sigma_-, J_+, J_-$</td>
</tr>
<tr>
<td>$\Gamma_4$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>$J_+, J_-$</td>
</tr>
<tr>
<td>$\Gamma_5$</td>
<td>2</td>
<td>-1</td>
<td>0</td>
<td>-2</td>
<td>1</td>
<td>$0, k_+, \sigma_+, J_+, \sigma_+, J_+, J_-$</td>
</tr>
<tr>
<td>$\Gamma_6$</td>
<td>2</td>
<td>-1</td>
<td>0</td>
<td>2</td>
<td>-1</td>
<td>0</td>
</tr>
</tbody>
</table>

where $k_\pm = k_x \pm ik_y$, $k_l^2 = k_x^2 + k_y^2$, $J_\pm = \frac{1}{\sqrt{2}}(J_x \pm iJ_y)$, $2[J_z, J_\pm] = J_z J_\pm + J_\pm J_z$, $\sigma_\pm = \frac{1}{2}(\sigma_x \pm \sigma_y)$.

### C. 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 $91^*$, and following criterions.

The criterion $k_F > \sqrt{n}/4$ at carrier densities $4 \times 10^{12}$ cm$^{-2}$, at a temperature $T=0$ K is carried as $1 > 0.1$. The ratio of Coulomb potential energy to the Fermi energy is $r_e = E_C/E_F = 0.63 < 1$. 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

![Absorption coefficient for the quantum well ZnO/Mg$_{0.27}$Zn$_{0.73}$O with a width 4 nm, at a carriers concentration $4 \times 10^{12}$ cm$^{-2}$, at a temperature 300 K.](image)
the longitudinal z direction on transversal in-plane wave function localization is less 1. We have compared the Hartree band gap with the flat band gap as well as the Hartree band gap with the Hartree-Fock band gap and have found $E_{\text{H}} - E_{\text{Flat band}} = 20.72 \text{ meV}$, $E_{\text{H}}^{\text{HF}} - E_{\text{H}} = 4.40 \text{ meV}$. An overlap integrals of the wave functions of holes and electron taking into account besides the piezoelectric effects the exchange-correlation effects in addition is greater than an overlap integral of Hartree ones. The Hartree particles distribute greater on edges of quantum well than Hartree-Fock particles. It is found that an effective mass of heavy hole of Mg$_{0.37}$Zn$_{0.73}$O under biaxial strain is greater than an effective mass of heavy hole of ZnO. It is calculated that an electron mass is less than a hole mass. It is found that the Bohr radius is greater than the localization range particle-hole pair, hence the excitons may be spontaneously created.

III. PARTICLE-HOLE PAIR INSTABILITY IN CARBON RIBBONS IN THE VICINITY OF DIRAC POINT

Fermi optical ground states of electron-hole pair in carbon ribbons in the vicinity of Dirac point are found. We found the analytical solutions from equation of motion for polarization operators within Hartree-Fock approximation. Particle-hole pair instability for supercritical Coulomb potential is predicted via resonant states with complex number energies. It signifies the existing the tachyon solutions in Whittaker equations of which can be well known the Heisenberg equations in one-dimensional systems.

The layered graphites present a new state of matter of layered materials $^{93-101}$. The energy bands for graphite was found using "tight-binding" approximation by P.R. Wallace. In the low-energy limit the single-particle spectrum is Dirac cone similarly to the light cone in relativistic physics, where the light velocity is substituted by the Fermi velocity $v_F = 10^6 \text{ m/s}$ and describes by the massless Dirac equation.

The graphene is the single graphite layer, i.e. two-dimensional graphite plane of thickness of single atom. The graphene lattice resembles a honeycomb lattice. The graphene lattice one can consider like into the composite of two triangular sublattices. In 1947 Wallace in "tight-binding" approximation consider a graphite which consist off the graphene blocks with taken into account the overlap only the nearest $\pi$-electrons.

The two-dimensional nature of graphene and the space and point symmetries of graphene acquire of the reason for the massless electron motion since lead into massless Dirac equation (Majorana fermions). At low-energy limit the single particle spectrum forms with $\pi$-electron carbon orbital and consist off completely occupation valence cone and completely empty conduction cone, which have cone like shape with single Dirac point. In Dirac point the existing an electron as well as a hole is proved. The state in Dirac cone is double degenerate with taken into account a spin.

The existing of the massless Dirac fermions in graphene was proved based on the unconventional quantum Hall effect. The reason of creation the integer Hall conductivity $^{104-107}$ is derived from Berry phase $^{108,109}$. When the magnetic field is applied perpendicularly into graphene plane the lowest $(n=0)$ Landau level has the energy $\pm \Delta$ in two nonequivalent cones $K_\pi$, correspondingly $^{110}$. In the paper $^{110}$ the Dirac mass via a splitting value is found when Zeeman coupling is absence. These properties of the lowest Landau level which distribute between particles and antiparticles in equal parts are base of the integer quantum Hall effect in graphene $^{110}$. For $n \geq 1$ an all Landau levels are fourfold degenerate. For $n = 0$ a states in both cones are twofold degenerate with energies $\pm \Delta$ with taken into account a spin $^{110}$.

In the paper $^{111}$ a chiral superconductivity from electron-electron repulsive in doped graphene in the $M$ point is predicted.

In the paper $^{11}$ a Magneto-Coulomb levels at a three-dimensional saddle point were found. The Schrödinger equation for the three-dimensional saddle surface geometry at the magnetic field is applied unconventionally was solved exactly in the paper $^{11}$ by reducing into one-dimensional Schrödinger equation.

In the paper $^{112}$ the exciton binding energy is scaled with the formed band gap when the magnetic field is applied and an exciton insulator transition in carbon nanotubes was not found and their THz application was predicted.

In the paper $^{113}$ in the UCoGe material the high-temperature superconductivity is connected with spin fluctuations and hence may be reduced by magnetic field is applied.

In the paper $^{114}$ we present a theoretical investigation of excitonic states as well as their wave functions in graphene and in materials with "Mexican hat" band structure dispersion as well as in zinc-blende GaN. An integral form of the two-dimensional Schrödinger equation of Kepler problem in momentum space is solved exactly by projection the two-dimensional space of momentum on the three-dimensional sphere in the paper $^{61}$.

The integral Schrödinger equation was analytically solved by the projection the three-dimensional momentum space onto the surface of a four-dimensional unit sphere by Fock in 1935 $^{62}$.

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
superconductivity.

If the exciton binding energy is greater than the flat band gap in narrow-gap semiconductor or semimetal then at sufficiently low temperature the insulator ground state is instable with respect to the exciton formation\textsuperscript{115–118}. And excitons may be spontaneously created. In a system undergo a phase transition into a exciton insulator phase similarly to Bardeen-Cooper-Schrieffer (BCS) superconductor. In a single-layer graphene (SLG) the electron-hole pairing leads to the exciton insulator states\textsuperscript{7, 115,118}.

In the paper an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with complex dispersion is analytically solved. A complex dispersions lead to fundamental difference in exciton insulator states and their wave functions.

We analytically solve an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with electron-hole symmetry of reflection.

For graphene in vacuum the effective fine structure parameter $r_s = \frac{e^2}{\kappa \hbar v_F \sqrt{2}} = 1.23$. For graphene in substrate $r_s = 0.77$, when the permittivity of graphene in substrate is estimated to be $\kappa = 1.6$\textsuperscript{119}. It means the prominent Coulomb effects\textsuperscript{120}.

It is known that the Coulomb interaction leads to the semimetal-exciton insulator transition, where gap is opened by electron-electron exchange interaction\textsuperscript{115,121–123}. The perfect host combines a small gap and a large exciton binding energy\textsuperscript{115,118}.

In graphene the existing of bound pair states are still subject matter of researches\textsuperscript{112,124–127}.

It is known\textsuperscript{128} in the weak-coupling limit\textsuperscript{129}, exciton condensation is a consequence of the Cooper instability of materials with electron-hole symmetry of reflection inside identical Fermi surface. The identical Fermi surfaces is a consequence of the particle-hole symmetry of massless Dirac equation for Majorana fermions.

In the our paper the particle-hole pair instability for supercritical Coulomb potential is predicted via resonant states with complex number energies. It signifies the existing the tachyon solutions in Whittaker equations of which can be well known the Heisenberg equations in one-dimensional systems. These one-dimensional systems one can be carbon armchair ribbons in the vicinity of Dirac point in his spectrum within massless Dirac fermions (Majorana fermions).

A. Fermi optical ground state of electron-hole pair and exciton instability in carbon ribbons in the vicinity of Dirac point

In the paper\textsuperscript{130} a theoretical study the both the quantized energies of excitonic states and their wave functions in gapped graphene and in monolayer of MoS\textsubscript{2} is presented. An integral two-dimensional Schrödinger equation of the electron-hole pairing for a particles with electron-hole symmetry of reflection is analytically solved. The solutions of Schrödinger equation in momentum space in gapped graphene and in the direct band monolayer of MoS\textsubscript{2} by projection the two-dimensional space of momentum on the three-dimensional sphere are found. We analytically solve an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with electron-hole symmetry of reflection and with strong spin-orbit coupling. In monolayer of MoS\textsubscript{2} as well as in single-layer graphene (SLG) the electron-hole pairing leads to the exciton insulator states. Calculating an integral two-dimensional Schrödinger equation of the electron-hole pairing for bilayer graphene, an exciton insulator states with a gap 3 meV are predicted. The particle-hole symmetry of Dirac equation of layered materials allows perfect pairing between electron Fermi sphere and hole Fermi sphere in the valence band and conduction band and hence driving the Cooper instability.

It is well known\textsuperscript{124} that the tachyonic instability can be considered as the fall into the center phenomenon. However in view of QED\textsuperscript{131} a ways of curing the instability in graphene are quite different from that in the case of the supercritical Coulomb center. Since the coupling constant in freely standing graphene is larger than 1 the quasielectron in graphene has the supercritical Coulomb charge. In the opinion\textsuperscript{124} this leads to the production of an electron-hole pair via the coupling hole into the initial quasielectron forming a bound state. Thus the process of creating pairs continues leading to the formation of exciton (chiral) condensate in the stable phase and as a result the quasiparticles acquire a gap. The exciton condensate formation resolves the problem of instability hence a gap generation should take place in a freely standing graphene making it an insulator.

In the paper\textsuperscript{132,133} a theoretical study the both the quantized energies of excitonic states and their wave functions in graphene is presented. An integral two-dimensional Schrödinger equation of the electron-hole pairing for a particles with electron-hole symmetry of reflection is exactly solved. The solutions of Schrödinger equation in momentum space in graphene by projection the two-dimensional space of momentum on the three-dimensional sphere are found exactly. We analytically solve an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with electron-hole symmetry of reflection. In single-layer graphene (SLG) the electron-hole pairing leads to the exciton insulator states. Quantized spectral series and light absorption rates of the excitonic states which distribute in valence cone are found exactly. If the electron and hole are separated, their energy is higher than if they are paired. The
specifies of a matter polarization where \( \hat{E} \) and \( \hat{h} \) are the annihilation and creation operators of an electron and a hole. The Coulomb interaction Hamiltonian for particles in the electron-hole representation one can seek in the form:

\[
\tilde{H}_{C} = \frac{1}{2} \sum_{q,k,k'} V(q) \hat{e}_{k+q}^{\dagger} \hat{e}_{k}^{\dagger} \hat{h}_{k+q} + \frac{1}{2} \sum_{q,k,k'} V(q) \hat{h}_{k+q}^{\dagger} \hat{h}_{k}^{\dagger} \hat{e}_{k+q}^{\dagger} \hat{e}_{k}^{\dagger} + \frac{1}{2} \sum_{q,k,k'} V(q) \hat{h}_{k+q}^{\dagger} \hat{h}_{k}^{\dagger} \hat{e}_{k+q} \hat{e}_{k} - \frac{1}{2} \sum_{q,k,k'} V(q) \hat{h}_{k+q} \hat{h}_{k} \hat{e}_{k+q}^{\dagger} \hat{e}_{k}^{\dagger} + \frac{1}{2} \sum_{q,k,k'} V(q) \hat{h}_{k+q} \hat{h}_{k} \hat{e}_{k+q} \hat{e}_{k}.
\]

(144)

Consider a particle under the ac electric field \( \mathbf{E} e^{-i \omega t} + c.c. \). Its dynamics is described a Hamiltonian \( \hat{H} = v_F (\hat{\sigma} \mathbf{p}) \), where \( \hat{\sigma} \) is a Pauli matrix. Then \( \frac{i \hbar}{\omega} \left\langle (\hat{\sigma})_{m,n} \mathbf{E}_{\omega} e^{-i \omega t} + c.c. \right\rangle \) is a Hamiltonian of a interaction of light and matter:

\[
\hat{H}_{I} = \sum_{k} \frac{i \hbar v_F}{\omega} \left\langle (\hat{\sigma})_{m,n} \mathbf{E}_{\omega} e^{-i \omega t} + c.c. \right\rangle (\hat{e}_{k}^{\dagger} \hat{e}_{k} - \hat{h}_{k}^{\dagger} \hat{h}_{k}).
\]

(145)

The Heisenberg equation for the average value of a certain physical magnitude \( O \), which corresponds to the operator \( \hat{O} \) can be written as follows

\[
 i \hbar \frac{d}{dt} \left\langle \hat{O} \right\rangle = \left\langle [\hat{O}, \hat{H}] \right\rangle.
\]

(146)

We derive the equation of motion for the mean value of the product \( \hat{p}_k = \hat{h}_{k} \hat{e}_{k} \) for a microscopic dipole, which specifies of a matter polarization

\[
 i \hbar \frac{d}{dt} \hat{p}_k = 2\Xi_k \hat{p}_k - (1 - 2n_k) \Omega_k,
\]

(147)

where

\[
\Xi_k = \hbar v_F k - 2 \sum_{k'} V(k - k') \hat{n}_{k'},
\]

(148)

\[
\Omega_k = \frac{i \hbar v_F}{\omega} (\hat{\sigma})_{m,n} \mathbf{E}_{\omega} e^{-i \omega t} + \sum_{k'} V(k - k') \hat{p}_{k'},
\]

(149)

\[
\hat{p}_k = \frac{f_k}{g_k}.
\]

(150)

Substituting Eqs. (148),(149),(150) into Eq. (147) one can find the following matrix equation:

\[
 i \hbar \frac{d}{dt} \left[ \begin{array}{c} f_k \\ g_k \end{array} \right] = \left[ \begin{array}{c} 2\Xi_k - (1 - 2n_k) \sum_{k'} V(k - k') \\ 2\Xi_k \end{array} \right] \frac{f_k}{g_k} - \left( 1 - 2n_k \right) \frac{i \hbar v_F}{\omega} \sigma_{11} \mathbf{E}_{\omega} e^{-i \omega t} \left[ \begin{array}{c} f_k \\ g_k \end{array} \right] - \left( 1 - 2n_k \right) \frac{i \hbar v_F}{\omega} \sigma_{22} \mathbf{E}_{\omega} e^{-i \omega t} \left[ \begin{array}{c} f_k \\ g_k \end{array} \right]
\]

(151)

which can be rewritten in the form:
Figure 15. (Color online) Single-particle spectrum of graphene for massless Dirac fermions (Majorana fermions).

Figure 16. (Color online) Single-particle spectrum of carbon armchair ribbon.

\[ \epsilon \begin{pmatrix} f_k \\ g_k \end{pmatrix} + \begin{pmatrix} (1 - 2\theta(\mu - \epsilon_f(k+q))) & \epsilon V_F \sigma_{11} \\ (1 - 2\theta(\mu - \epsilon_f(k+q))) & \epsilon V_F \sigma_{22} \end{pmatrix} \begin{pmatrix} f_k \\ g_k \end{pmatrix} \begin{pmatrix} 2\Xi_k \\ (1 - 2\theta(\mu - \epsilon_f(k+q))) \sum_{k'} V(k - k') \end{pmatrix} \begin{pmatrix} f_{k'} \\ g_{k'} \end{pmatrix} = 0. \]  

Under Fourier transform of the matrix equation (152) one can find the system of equations for the functions \( \psi \) and \( \phi \) in a dimensionless values in the form:

Figure 17. (Color online) Single-particle spectrum \( \epsilon = v_F f(k) \) of carbon armchair ribbon (the width of the ribbon is \( m = 5 \) unit cells) \(^{134} \).
\[ z' \frac{d\phi}{dz'} - \left( \frac{z'}{2} - \frac{1}{2} - \alpha \right) \phi + \frac{2}{\alpha} \psi = 0, \]  
(153)

\[ z' \frac{d\phi}{dz'} - \left( \frac{z'}{2} + \frac{1}{2} - \alpha \right) \phi + \frac{2}{\alpha} \psi = 0. \]  
(154)

Substituting \( \phi \) from the first equation into the second one we find the equation for the \( \psi \) function

\[ \frac{d^2 \psi}{dz'^2} + \left( -\frac{1}{4} - \frac{1}{z'} (1 + \frac{\alpha}{2}) + \frac{(\alpha^2 + \frac{\gamma^2}{\alpha^2} - \frac{1}{4})}{z'^2} \right) \psi = 0, \]  
(155)

where

\[ z' = \frac{z}{-\partial \psi}, \]  
(156)

of which is the well known Whittaker equation\textsuperscript{135–137}. Its general solution is in the form of Whittaker functions

\[ \psi = C_1 W_{\kappa,\mu}(z) + C_2 M_{\kappa,\mu}(z), \]  
(157)

where

\[ \kappa = -(1 + \frac{\alpha}{2}), \]  
\[ \mu^2 = \alpha^2 + \frac{\gamma^2}{\alpha^2} - \frac{1}{2}. \]  
(158)

For Whittaker functions can be written the following integral relation\textsuperscript{135–137}:

\[ \Gamma\left( \frac{1}{2} - \kappa + \mu \right) W_{\kappa,\mu}(z) = e^{-\frac{1}{2} z^{\mu + \frac{1}{2}}} \times \int_0^\infty e^{-zt} t^{-\frac{1}{2} - \kappa + \mu} (1 + t)^{-\frac{1}{2} + \kappa + \mu} dt, \]  
(159)

\[ W_{\kappa,\mu}(z) = e^{-z^{\kappa/2}} 2 F_0\left( \frac{1}{2} - \kappa + \mu, \frac{1}{2} - \kappa - \mu, -\frac{1}{z} \right), \]  
(160)

\[ \Gamma\left( \frac{1}{2} - \kappa + \mu \right) \Gamma\left( \frac{1}{2} + \kappa + \mu \right) M_{\kappa,\mu}(z) = 2^{-2\sigma} \Gamma(2\mu + 1) z^{\mu + \frac{1}{2}} \times \int_{-1}^1 e^{\frac{1}{2} zt} (1 - t)^{-\frac{1}{2} + \kappa + \mu} (1 + t)^{-\frac{1}{2} - \kappa + \mu} dt. \]  
(161)

In \( z > z_0 \) range for supercritical Coulomb potential the solution of Eq. (155) we seek in the form

\[ f = C_2^{\alpha} W_{\kappa,\mu}\left( \frac{2}{\alpha^2} z \right), \]  
(162)

In \( z < z_0 \) range for supercritical Coulomb potential the solution of Eqs. (153), (154) we seek as follows

\[ \psi = A_1 z J_{\mu + 1/2}\left( \frac{2}{\alpha^2} z \right), \]  
(163)

\[ \phi = A_2 \operatorname{sgn}\left( \frac{2}{\alpha^2} z \right) J_{\mu - 1/2}\left( \frac{2}{\alpha^2} z \right). \]  
(164)

Under continuity conditions\textsuperscript{36} one can find on \( z = z_0 \)
\[
\frac{W_{n,1/2}(\frac{\gamma}{\alpha})}{W_{n,1/2}(\frac{\pi}{2})} = \frac{k+1}{k+1},
\]

\(k = \frac{J_1(\frac{\gamma}{\alpha})}{J_0(\frac{\gamma}{\alpha})},\)

where we have considered the states with the orbital quantum number \(j = \frac{1}{2}\) concerning of \(nS_{1/2}\) states i.e. the lowest-energy state belong to them

\[
\epsilon = |e| e^{i\beta}.
\]

We analytically found the solution i.e. tachyon states within complex number quantized energies of the sought for equation (347) in the form:

\[
\ln(2|\epsilon|R) + i(\beta - \pi/2) \simeq 2\left\{\frac{J_0(\frac{\gamma}{\alpha})}{J_0(\frac{\pi}{2})} - \frac{1}{2}\psi(1 - \frac{1}{2}) - \frac{1}{1+n} - \frac{\pi n}{\nu}\right\},
\]

where we replace

\[
\mu \rightarrow i\nu.
\]

So we found the resonant states for electron-hole pair in considered materials in which the bound states dive into the lower continuum and determine by the complex number energies. Our results are in close agreement with Ref. 124.

In our paper the particle-hole pair instability for supercritical Coulomb potential is predicted via resonant states with complex number energies. It signifies the existing the tachyon solutions in Whittaker equations of which can be well known the Heisenberg equations in one-dimensional systems. These one-dimensional systems one can be carbon armchair ribbons in the vicinity of Dirac point in his spectrum within massless Dirac fermions (Majorana fermions).

\section*{B. Conclusions and discussions}

Fermi optical ground states of electron-hole pair in carbon ribbons in the vicinity of Dirac point are found. We found the analytical solutions from equation of motion for polarization operators within Hartree-Fock approximation. Particle-hole pair instability for supercritical Coulomb potential is predicted via resonant states with complex number energies. It signifies the existing the tachyon solutions in Whittaker equations of which can be well known the Heisenberg equations in one-dimensional systems.

The integral Schrödinger equation for a parabolic bands was analytically solved by the projection the three-dimensional momentum space onto the surface of a four-dimensional unit sphere by Fock in 1935 62. In integral form of the two-dimensional Schrödinger equation of Kepler problem in momentum space is solved exactly by the projection of the two-dimensional space of momentum on the three-dimensional sphere in the paper 61.

In graphene the existing of bound pair states are still subject matter of researches 138.

In the paper 139,140 the possibility of extremum loop or toroidal energy surfaces in wurtzite semiconductor is discussed. The Bychkov-Rashba model 141 describes the electron motion in two-dimensional system with applied electric potential gradient field perpendicularly to the plane of system.

This Rashba spin splitting causes the shifting of oppositely spin-polarized energy band by momentum \(q\) in opposite directions.

The Rashba and Dresselhaus spin-orbit couplings in GaAs quantum wells were studies in the paper 142.

The bismuth tellurohalides BiTeCl, BiTeBr, and BiTeI have hexagonal crystal structures and giant Rashba spin splitting in two-dimensional systems 143,144. These materials in the low-energy limit are described "Mexican hat" shape dispersion.

In the paper an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with complex dispersion is analytically solved. A complex dispersions lead to fundamental difference in exciton insulator states and their wave functions.
We analytically solve an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with electron-hole symmetry of reflection.

It is known that the Coulomb interaction leads to the semimetal-exciton insulator transition, where gap is opened by particle-particle exchange interaction. The perfect host combines a small gap and a large exciton binding energy.

We consider the pairing between oppositely charged particles in materials with a “Mexican hat” shape band structure dispersion or in materials with giant Rashba spin splitting and in graphene. The Coulomb interaction leads to the electron-hole bound states scrutiny study of which acquire significant attention in explanations of high-temperature superconductivity.

It is known if the exciton binding energy is greater than the flat band gap in narrow-gap semiconductor or semimetal then at sufficiently low temperature the insulator ground state is instable concerning to the exciton formation with follow up spontaneous production of excitons. In a system undergo a phase transition into an exciton insulator phase similarly to BCS superconductor. In a semiconductors with a “Mexican hat” shape band structure dispersion as well as in graphene the electron-hole pairing leads to exciton insulator states.

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The particle-hole symmetry of Dirac equation of layered materials allows perfect pairing between electron Fermi sphere and hole Fermi sphere in the valence band and conduction band and hence driving the Cooper instability. In the weak-coupling limit in graphene with the occupied conduction-band states and empty valence-band states inside identical Fermi surfaces in band structure, the exciton condensation is a consequence of the Cooper instability.

In the paper a theoretical study the both the quantized energies of excitonic states and their wave functions in gapped graphene and in monolayer of MoS$_2$ is presented. An integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with electron-hole symmetry of reflection is analytically solved. The solutions of Schrödinger equation in momentum space in gapped graphene and in the direct band monolayer of MoS$_2$ by projection the two-dimensional space of momentum on the three-dimensional sphere are found. We analytically solve an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with electron-hole symmetry of reflection and with strong spin-orbit coupling. In monolayer of MoS$_2$ as well as in single-layer graphene (SLG) the electron-hole pairing leads to the exciton insulator states. Calculating an integral two-dimensional Schrödinger equation of the electron-hole pairing for bilayer graphene, an exciton insulator states with a gap 3 meV are predicted. The particle-hole symmetry of Dirac equation of layered materials allows perfect pairing between electron Fermi sphere and hole Fermi sphere in the valence band and conduction band and hence driving the Cooper instability.

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In the our paper the particle-hole pair instability for supercritical Coulomb potential is predicted via resonant states with complex number energies. It signifies the existing the tachyon solutions in Whittaker equations of which can be well known the Heisenberg equations in one-dimensional systems. These one-dimensional systems one can be carbon armchair ribbons in the vicinity of Dirac point in his spectrum within massless Dirac fermions (Majorana fermions).

C. Mathematical appendix II

Factorizing the convolutions of operators with the help of the Wick theorem, one can derive Heisenberg equation for the polarization operator. The pairwise convolutions originate from the operators, which are taken at different points (i.e. within Hartree-Fock approximation):

\[ [\hat{h}_{+k} \hat{e}_{k'}, \hat{e}^\dagger_{k} \hat{e}_{k}] = \hat{h}_{+k} \hat{e}_{k'} \hat{e}^\dagger_{k} \hat{e}_{k} - \hat{e}^\dagger_{k} \hat{e}_{k} \hat{h}_{+k} \hat{e}_{k'}, \]  
(170)

\[ \hat{e}^\dagger_{k} \hat{e}_{k} \hat{h}_{+k} \hat{e}_{k'} = -\hat{h}_{+k} \hat{e}^\dagger_{k} \hat{e}_{k} \hat{e}_{k} = -\delta_{k,k'} \hat{h}_{+k} \hat{e}_{k} + \hat{h}_{+k} \hat{e}_{k'} \hat{e}^\dagger_{k}, \]  
(171)

\[ [\hat{h}_{+k} \hat{e}_{k'}, \hat{e}^\dagger_{k} \hat{e}_{k}] = -\delta_{k,k'} \hat{h}_{+k} \hat{e}_{k}, \]  
(172)

\[ [\hat{h}_{+k} \hat{e}_{k'}, \hat{h}^\dagger_{-k} \hat{h}_{-k}] = \hat{h}_{+k} \hat{e}_{k'} \hat{h}^\dagger_{-k} \hat{h}_{-k} - \hat{h}^\dagger_{-k} \hat{h}_{-k} \hat{h}_{+k} \hat{e}_{k'}, \]  
(173)

\[ \hat{h}^\dagger_{-k} \hat{h}_{-k} \hat{h}_{+k} \hat{e}_{k'} = -\delta_{k,k'} \hat{h}_{-k} \hat{e}_{k'} + \hat{h}_{-k} \hat{e}_{k'} \hat{h}^\dagger_{-k} \hat{h}_{-k} = -\delta_{k,k'} \hat{h}_{-k} \hat{e}_{k'}, \]  
(174)

\[ [\hat{h}_{-p} \hat{e}_{p}, \hat{e}^\dagger_{k+q} \hat{e}^\dagger_{k'} - q \hat{e}^\dagger_{k} \hat{e}_{k}] = \delta_{p,k+q} \hat{h}_{-p} \hat{e}^\dagger_{k+q} \hat{e}^\dagger_{k'} \hat{e}_{k} - \delta_{p,k'} - q \hat{p} \hat{e}^\dagger_{k} \hat{e}^\dagger_{k'+q} \hat{e}_{k'}, \]  
(175)

\[ [\hat{h}_{-p} \hat{e}_{p}, \hat{h}^\dagger_{-k+q} \hat{h}^\dagger_{k'} - q \hat{h}_{-k} \hat{e}_{k}] = \delta_{p,k+q} \hat{h}_{-p} \hat{h}^\dagger_{-k+q} \hat{h}^\dagger_{k'} \hat{e}_{k} - \delta_{p,k'} - q \hat{p} \hat{h}^\dagger_{k'} \hat{h}^\dagger_{-k+q} \hat{e}_{k'}, \]  
(176)

\[ [\hat{h}_{-p} \hat{e}_{p}, \hat{e}^\dagger_{k+q} \hat{h}^\dagger_{k'} - q \hat{h}_{-k} \hat{e}_{k'}] = \delta_{p,k+q} \hat{h}_{-p} \hat{e}^\dagger_{k+q} \hat{h}^\dagger_{k'} \hat{e}_{k'} - \delta_{p,k'} - q \hat{p} \hat{e}^\dagger_{k+q} h_{k'} \hat{e}_{k'}, \]  
(177)

\[ [\hat{h}_{-p} \hat{e}_{p}, \hat{h}^\dagger_{-k+q} \hat{h}^\dagger_{k'} - q \hat{h}_{-k} \hat{e}_{k'}] = \delta_{p,k+q} \hat{h}_{-p} \hat{h}^\dagger_{-k+q} \hat{h}^\dagger_{k'} \hat{e}_{k'} - \delta_{p,k'} - q \hat{p} \hat{h}^\dagger_{k'} \hat{h}^\dagger_{-k+q} \hat{e}_{k'}, \]  
(178)

\[ [\hat{h}_{-p} \hat{e}_{p}, \hat{e}^\dagger_{k+q} \hat{h}^\dagger_{k'} - q \hat{h}_{-k} \hat{e}_{k'}] = \delta_{p,k+q} \hat{h}_{-p} \hat{e}^\dagger_{k+q} \hat{h}^\dagger_{k'} \hat{e}_{k'} - \delta_{p,k'} - q \hat{p} \hat{e}^\dagger_{k+q} h_{k'} \hat{e}_{k'}, \]  
(179)

\[ [\hat{h}_{-p} \hat{e}_{p}, \hat{h}^\dagger_{-k+q} \hat{h}^\dagger_{k'} - q \hat{h}_{-k} \hat{e}_{k'}] = \delta_{p,k+q} \hat{h}_{-p} \hat{h}^\dagger_{-k+q} \hat{h}^\dagger_{k'} \hat{e}_{k'} - \delta_{p,k'} - q \hat{p} \hat{h}^\dagger_{k'} \hat{h}^\dagger_{-k+q} \hat{e}_{k'}, \]  
(180)

\[ [\hat{h}_{-p} \hat{e}_{p}, \hat{e}^\dagger_{k} \hat{h}^\dagger_{-k}] = \delta_{p,k+q} \hat{h}_{-p} \hat{h}^\dagger_{-k} - \delta_{p,k'} \hat{e}^\dagger_{k} \hat{e}_{p}, \]  
(181)
\[ [\hat{h}_p \hat{e}_p, \hat{h}_k \hat{e}_k] = 0, \]  
\[ (182) \]

\[ [\hat{h}_p \hat{e}_p, \hat{e}_k^\dagger \hat{e}_k] = \delta_{p,k} \hat{h}_p \hat{e}_k, \]  
\[ (183) \]

\[ [\hat{h}_p \hat{e}_p, \hat{h}^\dagger_k \hat{h}_k] = \delta_{p,k} \hat{h}_p \hat{e}_p, \]  
\[ (184) \]

\[ \begin{aligned}
\hbar^2 F (\hat{h}_p \hat{e}_p) &= v_F f(k) [\hat{h}_p \hat{e}_p, \hat{e}_k^\dagger \hat{e}_k + \hat{h}^\dagger_k \hat{h}_k] + \\
&+ \sum_k E_F [\hat{h}_p \hat{e}_p, \hat{e}_k^\dagger \hat{e}_k - \hat{h}^\dagger_k \hat{h}_k] + \\
&+ \frac{1}{2} \sum_{q,k,k'} V(q) [\hat{h}_p \hat{e}_p, \hat{e}_k^\dagger \hat{e}_k - \hat{h}^\dagger_k \hat{h}_k] + \\
&+ \frac{1}{2} \sum_{q,k,k'} V(q) [\hat{h}_p \hat{e}_p, \hat{e}_k^\dagger \hat{h}^\dagger_k \hat{h}^\dagger_k \hat{h}_k] + \\
&+ \frac{1}{2} \sum_{q,k,k'} V(q) [\hat{h}_p \hat{e}_p, \hat{e}_k^\dagger \hat{h}^\dagger_k \hat{h}^\dagger_k \hat{h}_k] + \\
&+ \frac{1}{2} \sum_{q,k,k'} V(q) [\hat{h}_p \hat{e}_p, \hat{e}_k^\dagger \hat{e}_k - \hat{h}^\dagger_k \hat{h}_k], \end{aligned} \]  
\[ (185) \]

\[ \begin{aligned}
\hbar^2 F (\hat{h}_p \hat{e}_p) &= v_F f(k) [\delta_{p,k} \hat{h}_p \hat{e}_k + \hat{h}_p \hat{e}_k] + \\
&+ \sum_k E_F [\delta_{p,k} \hat{h}_p \hat{e}_k - \hat{h}_p \hat{e}_k] + \\
&+ \frac{1}{2} \sum_{q,k,k'} V(q) [\delta_{p,k} \hat{h}_p \hat{e}_k + \hat{h}_p \hat{e}_k - \hat{h}_p \hat{h}_k] + \\
&+ \frac{1}{2} \sum_{q,k,k'} V(q) [\delta_{p,k} \hat{h}_p \hat{e}_k + \hat{h}_p \hat{h}_k - \hat{h}_p \hat{h}_k] + \\
&+ \frac{1}{2} \sum_{q,k,k'} V(q) [\delta_{p,k} \hat{h}_p \hat{e}_k + \hat{h}_p \hat{h}_k - \hat{h}_p \hat{h}_k], \end{aligned} \]  
\[ (186) \]

IV. OPTICAL POLARIZATION ANISOTROPY, INTRINSIC STARK EFFECT AND COULOMB EFFECTS ON THE LASING CHARACTERISTICS OF [0001]-ORIENTED GaN/Al_{0.3}Ga_{0.7}N QUANTUM WELLS

In this paper we present a theoretical investigation of space separated electron and hole distributions, which is reflected in self-consistent solving Schrödinger equations for electrons and holes and Poisson equation. The results are illustrated for the GaN/Al_{0.3}Ga_{0.7}N quantum well. The optical gain spectrum in [0001]-oriented GaN/Al_{0.3}Ga_{0.7}N quantum well in the ultraviolet region was calculated. It is found that both the matrix elements of optical transitions from the heavy hole band and optical gain spectrum have only the strict x (or y) light polarizations. We present studies of the influence of wave functions confinement on optical gain which is observed with an implicit dependence on the built-in electric field which is calculated to be 2.3 MV/cm. Whereas structures with narrow well widths exhibit the
usual dependent developing of the light gain maximum almost without shifting spectral region, a significant blueshift of the gain maximum is found with increasing plasma density for wider quantum wells. This blueshift is ascribed to the interplay between the screening of a strain induced piezoelectric field and bandstructure. A large Sommerfeld or Coulomb enhancement is present in the quantum well.

Direct wide band gap group III-nitride semiconductors based on GaN and its alloys have received great attention due to their applications in optoelectronic devices such as light-emitting diodes and lasers at green-blue and near-ultraviolet wavelengths, solar-blind photodetectors. A number of ultraviolet light-emitting diodes and laser diodes already have been demonstrated. Realizing deep-ultraviolet semiconductor-based light-emitting diodes will provide compact, high-efficiency light sources for various applications, for example in biological detections and data storage. Thus, these structures are in the developmental stage.

In this paper we present a theoretical investigation of the intricate interplay of the electron-hole plasma with the built-in electric field. For this purpose the quantum well bandstructure calculation is performed using invariant method and the envelope approximation. We consider the quantum well GaN of width \( w \), which is oriented perpendicular to the growth direction (0001) and localized in the spatial region \(-w/2 < z < w/2\). In GaN/AlGaN 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 \( \varepsilon \) in wurtzite structures.

The wave functions confinement has a strong influence on optical gain which is observed with an implicit dependence on the built-in electric field which is calculated to be 2.3 MV/cm. Such fields are present in GaN/Al\(_{0.3}\)Ga\(_{0.7}\)N systems because the strain is induced lattice mismatch. The relative magnitude of piezoelectric effects depends sensitively on quantum-well width and plasma density. In this paper we present a theoretical investigation of space separation of electron and hole distributions, which is reflected in self-consistent solving Schrödinger equations for electrons and holes and Poisson equation. The Poisson equation contains Hartree potential which takes into considerations space distributions of charge density for electrons and holes. The details of the bandstructure has to be included, because we are comparing different quantum well structures. Also discussed in this paper is the treatment of the quantum confined Stark effect (QCSE) in the band structure calculations in high concentration regime.

By comparing the gain spectra for two GaN/AlGaN quantum well structures of different well width, we show the interplay of bandstructure and piezoelectric effect. In particular, we see in wide quantum well structures, where the QCSE is appreciable a significant blueshift of the gain maximum, while structures with narrow well width exhibit the usual dependent developing of the light gain maximum almost without shifting spectral region.

A similar blueshifts of the exciton resonance also was observed and microscopically analyzed for GaInN/GaN quantum well systems. They reflect a perturbation of the compensation between self-energy and field renormalization contributions to the microscopic interband polarization by real space charge separation. Such feature is present in this quantum well, that is not inherently for the GaAs quantum well for lack of piezoelectric field. Accounting of Coulomb renormalization of momentum matrix element in two-band model of quantum well structure causes of variation in oscillator strength with variation of carrier density and quantum well configuration.

In paper, both the interband momentum matrix elements and the optical gain of strained wurtzite GaN quantum well were presented without including the intrinsic built-in piezoelectric field in quantum well structure.

In paper, laser gain was investigated for AlGaN wurtzite quantum well structures. The optical gain spectra for a wurtzite quantum well were computed by simultaneously diagonalizing the kp Hamiltonian and solving Poisson’s equation. But a significant shift of the gain maximum with increasing plasma density in the framework of single well were presented without including the intrinsic built-in piezoelectric field in quantum well structure. This result coincides with the our gain calculations in Fig. 22.

In paper, a self-consistent calculation of optical gain was presented in pseudomorphically strained GaN quantum wells as a function of carrier density. But in the paper was not accounted the spectrum renormalization and electric dipole moment which are caused by electron-electron and electron-hole Coulomb correlations.

Understanding the influence of bandstructure and QCSE on laser gain properties should help towards improving the laser performance and optimal device configurations.

The light gain spectrum presented in the paper reflects only strict TE (\( x, \) or \( y \)) light polarization. Because, it is known that the valence-band spectrum at the \( \Gamma \) points originates from sixfold degenerate \( \Gamma_{15} \) state. 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.

In Paper to describe the emission or absorption processes the energies, as well as the wave functions of the lowest conduction subband and the valence subbands are calculated. The quantum well width and charge density dependence of both the matrix elements for dipole optical interband transitions, and the light gain spectrum in GaN quantum wells are derived. Section presents Hartree-Fock light gain spectra, matrix elements for dipole optical interband transitions that are calculated with the theory described in Paper. By comparing the light gain spectra for two GaN/AlGaN quantum well structures of different well widths, we show the interplay of bandstructure, polarization field, and charge density. It is found the red renormalization of light gain spectrum caused the electron-electron and hole-hole Coulomb...
interactions. It is found, that Sommerfeld enhancement composes 26.7 percent relatively the gain value, which was obtained in Hartree problem. This enhancement of electric dipole momentum is caused by electron-hole Coulomb interaction of attraction.

A. Theory

We consider QCSE in strained würtzite GaN/Al$_{0.3}$Ga$_{0.7}$N quantum wells with widths 2.6 nm and 3.9 nm, in which barrier height is finite, constant value for electrons and is equal $U_0 = 490$ meV. Theoretical analysis of consideration of optical gain of strained würtzite quantum well lasers is based on self-consistent solving Schrödinger equations for electrons and holes in quantum well of width $w$ with including Stark effect and Poisson equation. The Poisson equation contains Hartree potential which takes into consideration charge density for electrons and holes. All researches are performed at the temperature 300K.

The first energy level of electron in quantum well of width $w$ is equal

$$E_1 = \frac{2\ell^2 \hbar^2}{m w^2},$$  \hspace{1cm} (188)

where $m = 0.19m_0$ - is an electron effective mass, $\xi$ is found from equation

$$\cos \xi = \pm \gamma,$$

where $\gamma = \frac{\hbar}{\pi} \sqrt{\frac{2}{2mU_0}}$, tan $\xi > 0$, $\xi = \frac{k_0 w}{2}$. For $k_0$ the next equality is performed:

$$\arcsin \frac{\hbar k_0}{\sqrt{2mU_0}} = \frac{n\pi - k_0 w}{2},$$  \hspace{1cm} (190)

The wave function of electron of first energy level with accounts QCSE is equal

$$\psi_0 = \frac{1}{\sqrt{\Lambda}} e^{ik_\rho z}\psi(z, \beta)|S|\sigma_c),$$

where

$$\psi(z, \beta) = \begin{cases} 
\psi_1(z, \beta) \\
\psi_2(z, \beta) \\
\psi_3(z, \beta).
\end{cases}$$

where $\psi_1(z, \beta) = C_1 e^{(\kappa_0 - \beta)(z + \frac{w}{2})}$, $\psi(z, \beta) = C \sin (k_0 z + \delta_0) e^{-\beta z}$, $\psi_2(z, \beta) = C_2 e^{-(\kappa_0 + \beta)(z - \frac{w}{2})}$. From bond conditions $\psi_1(z, \beta)|_{z=-w/2} = \psi(z, \beta)|_{z=-w/2}$, $\psi_2(z, \beta)|_{z=w/2} = \psi(z, \beta)|_{z=w/2}$, $\psi_3(z, \beta)|_{z=-w/2} = \psi(z, \beta)|_{z=-w/2}$. One can find $C_1 = C \sin (-\frac{k_0 w}{2} + \delta_0) e^{\beta w}$, $C_2 = C \sin (\frac{k_0 w}{2} + \delta_0) e^{-\beta w}$, $\kappa_0 = k_0 (1 - \cos \frac{k_0 w}{2})$, $\delta_0 = \frac{k_0 w}{2} + \arctan \frac{\gamma_\xi}{\kappa_0}$, where $\Lambda$ is the area of the quantum well in the $xy$ plane, $p_0$ 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:

$$\int_{-\infty}^{\infty} |\psi(z, \beta)|^2 dz = 1.$$  \hspace{1cm} (193)

In the such writing form of wave function is reflected information, that the conduction band is corresponded $\Gamma_7$ representation, which arises in consequence of crystal field splitting from $\Gamma_1$, $C_{\Gamma_7}$ space group, that is conduction band wave functions originate from $S$ atomic orbital. This is important at momentum matrix elements derivation using Wigner-Eckart theorem.

The strong lattice mismatch in GaN and Al$_{0.3}$Ga$_{0.7}$N leads to internal strain in würtzite layer GaN. In noncentrosymmetric structures the internal strain can induce a macroscopic built-in polarization field. This phenomenon is known as the piezoelectric effect. This phenomenon is also be described as a strain inducing an electric field. It is known, that this piezoelectric field, which is perpendicular to the quantum well plane may be appreciable because of
Figure 18. (Color online) Calculated square of the wave functions of a heavy hole (hh) and a light hole (lh) at the transverse wave vector $k_t = 8 \times 10^6 \text{cm}^{-1}$ and an electron (c) (a); the charge density distribution on the quantum well of width of 3.9 nm (b) at the charge concentration $9 \times 10^{12} \text{cm}^{-2}$.

Figure 19. (Color online) Effective screening electric field distribution (c); the quantum well potential and screening potential on the quantum well of width of 3.9 nm (d) at the charge concentration $9 \times 10^{12} \text{cm}^{-2}$.

the large piezoelectric constant in würtzite structures which are connected:

$$E = -\frac{4\pi}{\kappa}(\varepsilon_{31} - \varepsilon_{33})C_{13}\varepsilon_{xx} + P_{sp},$$  

(194)

where $\varepsilon$-is piezotensor, $P_{sp}$-spontaneous polarization, $\varepsilon$- strain tensor, $C_{13}, C_{33}$- elastic constant, $\kappa$- the permittivity of the host materials. It is calculated the built-in piezoelectric field in GaN/Al$_{0.3}$Ga$_{0.7}$N quantum well structure from (194) and found $E \simeq 0.23 \times 10^7 \text{ V/cm}$.

We assume following values for constants $C_{13} = 106 \text{ GPa}$, $C_{33} = 398 \text{ GPa}$, $\varepsilon_{31} = -0.44 \times 10^8 \text{ V/cm}$, $\varepsilon_{33} = 0.66 \times 10^8 \text{ V/cm}$, $P_{sp} = -0.26 \times 10^7 \text{ V/cm}$. The transverse component of the biaxial strain are proportional to the difference between the lattice constants of material of well and barrier and depend on Al content: $x$, $\varepsilon_{xx} = \varepsilon_{yy} = \frac{a_{Al_xGa_{1-x}N} - a_{GaN}}{a_{GaN}}$, $a_{Al_xGa_{1-x}N} = a_{GaN} + x(a_{AlN} - a_{GaN})$; $a_{AlN} = 0.31892 \text{ nm}$, $a_{AlN} = 0.3112 \text{ nm}$. The longitudinal component of deformation is expressed through elastic constants and transverse component of deformation: $\varepsilon_{zz} = -2\varepsilon_{xx}\varepsilon_{zz}$.

One can find the functional, which is built from (191,192) in the form:

$$J(\beta) = \frac{\langle \Psi|\hat{H}|\Psi \rangle}{\langle \Psi|\Psi \rangle},$$  

(195)
Figure 20. (Color online) Moment matrix elements for the $x$- (or $y$-) polarization (a) and the $z$-polarization (b): (1(a),2(a)) quantum well of width of 3.9 nm at the concentration $n = p = 9 \times 10^{12} \text{cm}^{-2}$; (1(a),2(a)) quantum well of width of 3.9 nm at the concentration $n = p = 7 \times 10^{12} \text{cm}^{-2}$; (1(b),2(b)) quantum well of width of 2.6 nm at the concentration $n = p = 9 \times 10^{12} \text{cm}^{-2}$; (1(b),2(b)) quantum well of width of 2.6 nm at the concentration $n = p = 7 \times 10^{12} \text{cm}^{-2}$.

where

$$H = H_c - \frac{\hbar^2}{2m_e^*} \frac{\partial^2}{\partial z^2} + V(z),$$

(196)

where $V(z) = U(z) + e\Phi(z)$,

$$H_c = E_g + \Delta_1 + \Delta_2 + \frac{\hbar^2}{2m_e^*}k^2 + a_{e\perp}e_{zz} + a_{e\perp}(\epsilon_{xx} + \epsilon_{yy}),$$

(197)

$m_{z,\perp} = 0.19m_0$, $a_{e\perp} = -4080\text{meV}$ 167. $U(z)$ can be represented in the form:

$$U = \begin{cases} U_0 - \frac{eE_w}{2}, z \in (-\infty, -w/2) \\ eE_z, z \in [-w/2, w/2] \\ U_0 + \frac{eE_w}{2}, z \in (w/2, \infty) \end{cases}$$

(198)

To account the piezoelectric effects, we modify the Schrödinger equation for electrons and holes by including an off-diagonal contribution to the electron and hole Hamiltonian. Schrödinger equation for infinitely deep quantum well with including QCSE and Hartree potential which is created by space separated electrons and holes may be presented in the form:

$$\hat{H}\Psi_\nu(r) = E_\nu\Psi_\nu(r),$$

(199)

where $\hat{H} = \hat{H}_+ + eE_z + e\Phi(z)$. We introduce the Bloch function written as vector in the three-dimensional Bloch space:

$$|\alpha \sigma \nu, k_t\rangle = \begin{bmatrix} \phi_1^{(1)}(z, k_t) \\ \phi_1^{(2)}(z, k_t) \\ \phi_1^{(3)}(z, k_t) \end{bmatrix} \begin{bmatrix} |1, \sigma \nu\rangle \\ |2, \sigma \nu\rangle \\ |3, \sigma \nu\rangle \end{bmatrix},$$

(200)

where

$$\phi_\alpha^{(j)} = \sum_{i=1}^n V_{k_t}^{(j)}[i, \alpha] \chi_i(z),$$

(201)
and \( j = 1, 2, 3 \). The Bloch vector of \( \alpha \)-type hole with spin \( \sigma_v = \pm \) and momentum \( k_t \) is specified by its three coordinates \( [V_{k_t}^{(1)}|n, \alpha], V_{k_t}^{(2)}|n, \alpha], V_{k_t}^{(3)}|n, \alpha] \) in the basis \([1, \sigma_v], [2, \sigma_v], [3, \sigma_v])\). 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

\[
\chi_n(z) = \sqrt{\frac{2}{w}} \sin \left( \pi n \left( \frac{z}{w} + \frac{1}{2} \right) \right),
\]

(202)

where \( n \) is a natural number. The hole wave function can be written as

\[
\Psi_{\nu}^{\alpha\sigma_v}(r) = \frac{e^{ik_t r}}{\sqrt{S}} |\alpha \sigma_v k_t>,
\]

(203)

where \( \nu = \{k_t, \alpha\} \), in the envelope-wave approximation: approximation in which wave function is considered as product of envelope part \( \chi(z)e^{ikt} \) and periodical Bloch multiplier. Bloch vectors in envelope wave approximation are projections of exact Bloch vectors on vectors subspace with \( \Gamma \) point inherent symmetry. The Hamiltonian in envelope wave approximation is

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

(204)

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

\[
F = \Delta_1 + \Delta_2 + \lambda + \theta,
\]

\[
G = \Delta_1 - \Delta_2 + \lambda + \theta,
\]

\[
\lambda = \lambda_k + \lambda_r,
\]

\[
\theta = \theta_k + \theta_r,
\]

\[
\lambda_k = \frac{\hbar^2}{2m_0}(A_1k_z^2 + A_2k_t^2),
\]

\[
\lambda_r = D_1\epsilon_{zz} + D_2(\epsilon_{xx} + \epsilon_{yy}),
\]

\[
\theta_k = \frac{\hbar^2}{2m_0}(A_3k_z^2 + A_4k_t^2),
\]

\[
\theta_r = D_3\epsilon_{zz} + D_4(\epsilon_{xx} + \epsilon_{yy}),
\]

\[
K_t = \frac{\hbar^2}{2m_0}(A_5k_t^2),
\]

\[
H_t = \frac{\hbar^2}{2m_0}(A_6k_1k_z),
\]

\[
\Delta = \sqrt{2}\Delta_3.
\]
\[ k_1^2 = k_x^2 + k_y^2, \]
\[ |1, \pm \rangle = \frac{1}{\sqrt{2}} [|1, 1\rangle | \uparrow \rangle e^{-\frac{i\pi}{4}} e^{-\frac{i\pi}{4}} \pm |1, -1\rangle | \downarrow \rangle e^{\frac{i\pi}{4}} e^{\frac{i\pi}{4}}], \]
\[ |2, \pm \rangle = \frac{1}{\sqrt{2}} [|1, 1\rangle | \downarrow \rangle e^{\frac{i\pi}{4}} e^{-\frac{i\pi}{4}} + |1, -1\rangle | \uparrow \rangle e^{\frac{i\pi}{4}} e^{\frac{i\pi}{4}}], \]
\[ |3, \pm \rangle = \frac{1}{\sqrt{2}} [|1, 0\rangle | \uparrow \rangle e^{\frac{i\pi}{4}} e^{-\frac{i\pi}{4}} + |1, 0\rangle | \downarrow \rangle e^{\frac{i\pi}{4}} e^{\frac{i\pi}{4}}], \]
\[ |1, 1\rangle = -\frac{1}{\sqrt{2}} |X + iY\rangle, \]
\[ |1, 0\rangle = |Z\rangle, \]
\[ |1, -1\rangle = \frac{1}{\sqrt{2}} |X - iY\rangle. \]

The valence subband structure \( E_\alpha^\sigma_z (k_z) \) can be determined by solving equations system:

\[
\sum_{j=1}^{3} \mathcal{H}_{ij}^\sigma_z (k_z = -i \frac{\partial}{\partial z} + \delta_{ij} E_\alpha^\sigma_z (k_i)) g_\alpha^{(j)\sigma_z} (z, k_i) = 0, \tag{205}\]

where \( i = 1, 2, 3 \). In the quasicubic approximation the effective mass parameters and deformation potential parameters take the form \( 164, 165 \):

\[
4A_5 - \sqrt{2} A_6 = A_3, 2A_4 = -A_1 = A_1 - A_2, \]
\[
4D_5 - \sqrt{2} D_6 = D_3, 2D_4 = -D_3 = D_1 - D_2, \]
\[
\Delta_2 = \Delta_3. \tag{206}\]

We assume in calculations for valence band effective-mass parameters \( 166 \): \( A_1 = -6.56, A_2 = -0.91, A_3 = 5.65, A_4 = -2.83, A_5 = -3.13, A_6 = -4.86 \), for deformation potentials \( 87 \): \( D_1 = 700\text{meV}, D_2 = 2100\text{meV}, D_3 = 1400\text{meV}, D_4 = -700\text{meV} \), for energy parameters at 300\( K \) \( 166, 167 \): \( E_g = 3507\text{meV}, \Delta_1 = \Delta_{so} = 16\text{meV}, \Delta_2 = \Delta_3 = \Delta_{so}/3 = 4\text{meV} \).

Solving Poisson equation with the condition \( \int_{-\infty}^{\infty} \rho(z) dz = 0 \):

\[
\frac{d^2 \Phi}{dz^2} = \frac{4\pi}{\kappa} \rho(z), \tag{207}\]

and with selected wave functions one can find a solution for Hartree potential \( e\Phi(z) \):

\[
e\Phi = \frac{2e^2}{\kappa} \sum_{\alpha, n, k_i} g_{\alpha} \int k_i dk_i \langle v_i, \sigma_v | V_{k_i}^z | \alpha, n | V_{k_i}^z | \alpha, k \rangle \sigma_v, v_i \rangle f_{\alpha, p}(k_i) \]
\[
\ast \left( \frac{w(\cos \pi Z(k+n)) - \cos \pi Z(n-k))}{\pi(n-k)^2} \right) \]
\[
\ast \left( \frac{w(\frac{Z}{2} + \frac{1}{4} \pi n \alpha Z)}{\pi(n-k)^2} \right) \]
\[
-\frac{2e^2}{\kappa} \int k_i dk_i \langle S | \langle \sigma_v | C | \sigma_v \rangle | S \rangle f_{\alpha, p}(k_i) \]
\[
\frac{1 - \cos(\beta w) \cos \frac{\pi}{4} \sin \frac{\pi}{4} (z + \frac{\beta}{2})}{4(\alpha \beta)^2} k_0^0 \beta \]
\[
\frac{2 \cos(2(\beta w) \cos \frac{\pi}{4} \sin \frac{\pi}{4} (z + \frac{\beta}{2}))}{4(\beta w)^2 + 4k_0^2} \]
\[
\frac{\sin(2(\beta w) \cos \frac{\pi}{4} \sin \frac{\pi}{4} (z + \frac{\beta}{2}))}{4(\beta w)^2 + 4k_0^2} \]
\[
= \frac{1 - \cos(\beta w) \cos \frac{\pi}{4} \sin \frac{\pi}{4} (z + \frac{\beta}{2})}{\beta w} e^{2(\cos \frac{\pi}{4} \sin \frac{\pi}{4} (z + \frac{\beta}{2}))} \frac{\sin(2(\beta w) \cos \frac{\pi}{4} \sin \frac{\pi}{4} (z + \frac{\beta}{2}))}{\beta w} e^{2(\cos \frac{\pi}{4} \sin \frac{\pi}{4} (z + \frac{\beta}{2}))}, \tag{208}\]

where \( Z = \frac{\pi}{2} + \frac{1}{2}, g_{\alpha} \) reflects degeneration of \( \alpha \) hole band, \( g_1 \) reflects degeneration of first quantized conduction band, \( e \) is the magnitude of the electron charge, \( \kappa \) is the permittivity of the host material, \( f_{\alpha, p}(k_i), f_{\alpha, p}(k_i) \) are the Fermi-Dirac distributions for holes and electrons. Here we assume charge concentrations \( 9 \times 10^{12}\text{cm}^{-2} \), and
Figure 21. (Color online) Calculated Hartree gain spectrum: (1(b)) quantum well of width of 3.9 nm at the concentration \( n = p = 9 \times 10^{12} \text{ cm}^{-2} \); (2(b)) quantum well of width of 3.9 nm at the concentration \( n = p = 7 \times 10^{12} \text{ cm}^{-2} \); (1(a)) quantum well of width of 2.6 nm at the concentration \( n = p = 9 \times 10^{12} \text{ cm}^{-2} \); (2(a)) quantum well of width of 2.6 nm at the concentration \( n = p = 7 \times 10^{12} \text{ cm}^{-2} \).

Solving (199) for holes in infinitely deep quantum well and finding minimum of functional (195) for electrons in quantum well with barriers of finite height may be found the both energy and wave functions of electrons and holes with including space distribution of electron and hole charge density in quantum well of given concentration in piezoelectric field. The screening field is determined by iterating Eq. (195), (199), (208) and the solutions to bandstructure calculation until convergence is reached. We use the space carrier distribution lowest order of electron and hole wave functions envelope.

Consider the matrix elements of interband transitions:

\[
M_{j\sigma \rightarrow j'\sigma'}(\mathbf{k}) = \int d^3r U_{j'\sigma' \mathbf{k}} \mathbf{e} \cdot \mathbf{p} U_{j\sigma \mathbf{k}}. \tag{209}
\]

The wave functions of valence band transforms according to the representation \( \Gamma_1 + \Gamma_5 \), while the wave function of conduction band transforms according to the representation \( \Gamma_1 \). In order to find the representation according to which transforms \( M_{j\sigma \rightarrow j'\sigma'}(\mathbf{k}) \), let to consider direct product \( \Gamma_1 \times (\Gamma_1 + \Gamma_5) \). Symmetry elements of point group \( C_{6v} \):

\[
g = E, C_2, 2C_3, 2C'_6, 3\sigma_v, 3\sigma'_v, \tag{210}
\]

where \( C_n \)-axis of \( n \) order, \( 3\sigma_v, 3\sigma'_v \)-6 planes of reflection which pass through axis of sixth order. For these elements one can find the representation \( \Gamma_1 + \Gamma_5 \):

\[
\chi(E) = 3, \chi(C_2) = -1, \chi(2C_3) = 0,
\]

\[
\chi(2C'_6) = 2, \chi(3\sigma_v) = 1, \chi(3\sigma'_v) = 1. \tag{211}
\]

The squares of irreducible representation elements are equal:

\[
g^2 = E, E, C_3, C_3, E, E. \tag{212}
\]

Let to find

\[
\chi^2_{\phi}(E) = 9, \chi^2_{\phi}(C_2) = 1, \chi^2_{\phi}(2C_3) = 0,
\]

\[
\chi^2_{\phi}(2C'_6) = 4, \chi^2_{\phi}(3\sigma_v) = 1, \chi^2_{\phi}(3\sigma'_v) = 1, \tag{213}
\]

while

\[
\chi^2_{\psi}(E^2) = 3, \chi^2_{\psi}(C_2^2) = 3, \chi^2_{\psi}(2C'_6^2) = 0,
\]

\[
\chi^2_{\psi}(2C_3^2) = 0, \chi^2_{\psi}(3\sigma_v^2) = 3, \chi^2_{\psi}(3\sigma'_v^2) = 3. \tag{214}
\]
Figure 22. (Color online) Calculated Hartree-Fock gain spectrum for the quantum well of width of 2.6 nm and at concentrations: \( n = p = 7 \times 10^{12} \text{ cm}^{-2} \) (Curve 1) and \( n = 9 \times 10^{12} \text{ cm}^{-2} \) (Curve 2).

Symmetric representation can be found in the form:

\[
\begin{align*}
\frac{1}{2}(\chi^2_v(g) + \chi_v(g^2)) : \\
\frac{1}{2}(\chi^2_v(E) + \chi_v(E^2)) = 6, \\
\frac{1}{2}(\chi^2_v(C_2) + \chi_v(C_2^2)) = 2, \\
\frac{1}{2}(\chi^2_v(2C_3) + \chi_v(2C_3^2)) = 0, \\
\frac{1}{2}(\chi^2_v(2C_6) + \chi_v(2C_6^2)) = 2, \\
\frac{1}{2}(\chi^2_v(3\sigma_v) + \chi_v(3\sigma_v^2)) = 2, \\
\frac{1}{2}(\chi^2_v(3\sigma_v') + \chi_v(3\sigma_v'^2)) = 2.
\end{align*}
\] (215)

Antisymmetric representations are equal:

\[
\begin{align*}
\frac{1}{2}(\chi^2_v(g) - \chi_v(g^2)) : \\
\frac{1}{2}(\chi^2_v(E) - \chi_v(E^2)) = 3, \\
\frac{1}{2}(\chi^2_v(C_2) - \chi_v(C_2^2)) = -1, \\
\frac{1}{2}(\chi^2_v(2C_3) - \chi_v(2C_3^2)) = 0, \\
\frac{1}{2}(\chi^2_v(2C_6) - \chi_v(2C_6^2)) = 2, \\
\frac{1}{2}(\chi^2_v(3\sigma_v) - \chi_v(3\sigma_v^2)) = -1, \\
\frac{1}{2}(\chi^2_v(3\sigma_v') - \chi_v(3\sigma_v'^2)) = -1.
\end{align*}
\] (216)

The symmetric representation can be expanded on the irreducible representations \( 2A_1 + E_1 + E_2 \), while as antisymmetric on \( A_2 + E_1 \). Thus in the wurtzite Hamiltonian \( H(\epsilon, \mathbf{k}) \) must be included the even functions (with respect to time inversion), which transpose according \( 2A_1 + E_1 + E_2 \) and odd functions, which transpose according \( A_2 + E_1 \). 

Vector representation may be written as

\[
\begin{align*}
\chi_v(E) = 3, \chi_v(C_2) = -1, \chi_v(2C_3) = 0, \\
\chi_v(2C_6) = 2, \chi_v(3\sigma_v) = 1, \chi_v(3\sigma_v') = 1.
\end{align*}
\] (217)

and can be expanded on irreducible representations \( A_1 + E_1 \). The representation according to which transposes interband operator right can be expanded on

\[
\Gamma_1 \times (\Gamma_1 + \Gamma_3) = A_1 + E_1.
\] (218)

Thus the direct product of representations (218) reflects of existing nonzero matrix elements of electric dipole momentum of interband transitions because from these representations can be formed the vector representation.
The only nonzero matrix elements between the basis functions exist for z light polarization are forbidden to have the strict x (or y) light polarization for the transitions from the heavy hole band to the conduction band, while momentum matrix elements for interband transitions in GaN structures. The results which are presented in Fig. 20, 21, 22, testify about optical polarization anisotropy of matrix elements in wurtzite GaN quantum well. Since the valence band top originates from \( \Gamma \) of TE polarized of light for two widths of quantum well. Such behavior agrees with the calculations of the momentum matrix elements in wurtzite GaN quantum well. Since the valence band top originates from \( \Gamma \), \( \Gamma_7 \), \( \Gamma_7 \) irreducible representations. The results which are presented in Fig. 20, 21, 22, testify about optical polarization anisotropy of momentum matrix elements for interband transitions in GaN/Al\(_{0.3}\)Ga\(_{0.7}\)N quantum well structures.

Allowed matrix elements of electric dipole momentum \((S|\sigma|e^p|v_l, \sigma_v\rangle\) is found in the form:

\[
\begin{align*}
(S|\uparrow e^p|v_1, \pm \rangle & = \frac{1}{2} P_{\pm} e^{i\varphi} e^{-i\frac{2\pi}{4}} \sin \theta, \\
(S|\uparrow e^p|v_2, \pm \rangle & = \frac{1}{2} P_{\pm} e^{-i\varphi} e^{i\frac{2\pi}{4}} \sin \theta, \\
(S|\uparrow e^p|v_3, \pm \rangle & = \pm \frac{1}{2} P_{\pm} e^{i\varphi} e^{i\frac{2\pi}{4}} \cos \theta, \\
(S|\uparrow e^p|v_4, \pm \rangle & = \pm \frac{1}{2} P_{\pm} e^{-i\varphi} e^{-i\frac{2\pi}{4}} \sin \theta, \\
(S|\uparrow e^p|v_5, \pm \rangle & = \frac{1}{2} P_{\pm} e^{i\varphi} e^{i\frac{2\pi}{4}} \cos \theta.
\end{align*}
\]

\((219)\)

due to symmetry properties of the Bloch functions, where \( \hat{p}_\pm = \hat{p}_x \pm i \hat{p}_y \). Two momentum matrix elements constants can be defined as: \( P_{\pm} \equiv \langle S|\hat{p}_\pm|X\rangle \) and \( P_{\pm} \equiv \langle S|\hat{p}_\pm|Z\rangle \). Due to cylindrical symmetry the matrix element depends only to the difference \( \varphi = \varphi_E - \varphi_k \) between plane-projected angles of vectors \( e^P \) and \( k \). To simplify calculations, we assume \( \varphi_k = 0 \) and denote spherical angles of vector \( e^P \) by \( \varphi \) and \( \theta \). We consider the case of a hole wave vector parallel to the c axis. In this situation \( \varphi = 0 \) in our calculations, and vector \( e^P \) in spherical coordinate \( e = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta) \), while \( e^P = \frac{1}{2} \sin \theta (e^{i\varphi} \hat{p}_- + e^{-i\varphi} \hat{p}_+) + \hat{p}_z \cos \theta \). It is known that, the values of constants \( |P_{\pm,\pm}|^2 \) can be found from kp theory

\[
\frac{m_0}{m_{\pm,\pm}^{(e)}} = 1 + \frac{2}{m_0} \sum_{j \neq e} \frac{|(c|\hat{p}_{\pm,\pm}|j\rangle|^2}{E_{c} - E_{j}}
\]

\((220)\)

and from experimentally measured conduction band effective mass \( m_{\pm,\pm}^{(e)} = 0.19 m_0 \) and \( E_9 = 3.5 \) eV can be estimated as \( \frac{2|m_{\pm,\pm}|^2}{m_0} \sim 15 \) eV.

In Fig. 20 we show the k-dependence of the matrix elements of the quantum well. We see, that the matrix elements have the strict x (or y) light polarization for the transitions from the heavy hole band to the conduction band, while for z light polarization are forbidden. That is why light gain spectrums presented in Fig. 21, 22 reflect only gain of TE polarized of light for two widths of quantum well. Such behavior agrees with the calculations of the momentum matrix elements in wurtzite GaN quantum well. Since the valence band top originates from \( \Gamma \), \( \Gamma_7 \), \( \Gamma_7 \) irreducible representations. The results which are presented in Fig. 20, 21, 22, testify about optical polarization anisotropy of momentum matrix elements for interband transitions in GaN/Al\(_{0.3}\)Ga\(_{0.7}\)N quantum well structures.
The optical material gain \(^{60,167}\) can be calculated from Fermi golden rule:

\[
a_\alpha = \frac{\pi e^2}{\kappa e m_0 w \omega} \sum_{\sigma_e=\uparrow,\downarrow} \sum_{\sigma_h=+,\ldots} \sum_{m,\alpha} \int k_t dk_t \int \frac{d\theta}{2\pi} |\mathbf{e} M_{\alpha m,\alpha'}(k_t)|^2 \frac{f_{\alpha'}^c(k_t) - f_{\alpha m}^c(k_t)}{f_{\alpha'}^c(k_t) + f_{\alpha m}^c(k_t)} \frac{\hbar^2}{\mu(k_t)^2 + \Gamma(k_t)^2},
\]

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, \(f_{\alpha m}^c, f_{\alpha m}^v\) are the Fermi-Dirac distributions for electrons in the conduction and valence bands, \(\mathbf{e}\) is a unit vector of vector potential of electromagnetic field, \(E_{\sigma' \sigma m}^c(k_t)\) 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. We consider the electromagnetic wave, which propagates in plane of quantum well. The modal gain, which determines the threshold condition of a laser, is proportional to the material gain multiplied by the optical confinement factor \(\Gamma\), and on the number \(a\) of quantum wells: \(\alpha = a_\alpha \Gamma a\). We take \(\Gamma\), which is equal 0.01, \(a\) is equal 1 in the calculations.

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.

Using the expressions for the basis functions we obtain two scalar polarizations - dependent matrix elements of electric dipole moment. For TE-polarization \((\hat{e} = \hat{x}\) or \(\hat{y} \perp c\) axis), that is for light polarization with vector, which lies in plane of quantum well:

\[
\frac{|(M_\sigma)^{\alpha\beta}(k_t)|^2}{|\langle S_{\sigma\beta\alpha\beta}(X)\rangle|^2} = \frac{1}{4} \left\{ \langle \Psi_1(\beta) \rangle \sum_n V_{k_t}^1[n, \alpha] \chi_n \right\}^2 + \frac{1}{4} \left\{ \langle \Psi_1(\beta) \rangle \sum_n V_{k_t}^2[n, \alpha] \chi_n \right\}^2,
\]

for \(\sigma = +\),

\[
\frac{|(M_\sigma)^{\alpha\beta}(k_t)|^2}{|\langle S_{\sigma\beta\alpha\beta}(X)\rangle|^2} = \frac{1}{4} \left\{ \langle \Psi_1(\beta) \rangle \sum_n V_{k_t}^3[n, \alpha] \chi_n \right\}^2 + \frac{1}{4} \left\{ \langle \Psi_1(\beta) \rangle \sum_n V_{k_t}^4[n, \alpha] \chi_n \right\}^2,
\]

for \(\sigma = -\).

For TM-polarization \((\hat{e} = \hat{z}|c\) axis), that is for light polarization with vector, which is perpendicular to quantum well plane:

\[
\frac{|(M_\sigma)^{\alpha\beta}(k_t)|^2}{|\langle S_{\sigma\beta\alpha\beta}(Z)\rangle|^2} = \frac{1}{4} \left\{ \langle \Psi_1(\beta) \rangle \sum_n V_{k_t}^3[n, \alpha] \chi_n \right\}^2 + \frac{1}{4} \left\{ \langle \Psi_1(\beta) \rangle \sum_n V_{k_t}^4[n, \alpha] \chi_n \right\}^2,
\]

for \(\sigma = +\),

\[
\frac{|(M_\sigma)^{\alpha\beta}(k_t)|^2}{|\langle S_{\sigma\beta\alpha\beta}(Z)\rangle|^2} = \frac{1}{4} \left\{ \langle \Psi_1(\beta) \rangle \sum_n V_{k_t}^3[n, \alpha] \chi_n \right\}^2 + \frac{1}{4} \left\{ \langle \Psi_1(\beta) \rangle \sum_n V_{k_t}^4[n, \alpha] \chi_n \right\}^2,
\]

for \(\sigma = -\).

B. Results and Their Discussion

To describe the interplay of the bandstructure and polarization effects in the Hartree problem, we consider a 2.6 nm and 3.9 nm GaN/Al\(_{0.3}\)Ga\(_{0.7}\)N quantum well structures. In the quantum well of width 2.6 nm at a concentration of \(9 \times 10^{12}\) cm\(^{-2}\), a optical gain maximum is equal 23673.7 cm\(^{-1}\) at a wavelength of \(\lambda = 334.5\) nm, while at a concentration of \(7 \times 10^{12}\) cm\(^{-2}\), a optical gain maximum is equal 14245.9 cm\(^{-1}\). Such gain is observed at a wavelength of \(\lambda = 336\) nm. In the quantum well of width 3.9 nm at a concentration of \(9 \times 10^{12}\) cm\(^{-2}\), a optical gain maximum is equal 5752.7 cm\(^{-1}\) at a wavelength of \(\lambda = 348.3\) nm, while at a concentration of \(7 \times 10^{12}\) cm\(^{-2}\), a optical gain maximum is equal 2840.8 cm\(^{-1}\). Such gain is calculated at a wavelength of \(\lambda = 352.1\) nm. Thus the optical gain in GaN/Al\(_{0.3}\)Ga\(_{0.7}\)N quantum well develops in the ultraviolet spectral region as shown in Fig. 21.

Numerically solving the Schrödinger equations (195, 199) for electrons and holes and Poisson equation (207), for the steady state solutions yields the square of wave functions of heavy hole (1), light hole (2) for example at the transverse wave vector \(k_t = 8 \times 10^6\) cm\(^{-1}\) and electron (3) a; the charge density distribution on the quantum well width (b); the effective screening electric field distribution (c); the quantum well potential and screening potential on the quantum well width (d). Such calculation results are present for concentration: \(9 \times 10^{12}\) cm\(^{-2}\), for 3.9 nm quantum well, which are shown in Fig. 18,19, and Hartree gain spectrums are shown in Fig. 21. For the narrow quantum well we see that at the \(7 \times 10^{12}\) cm\(^{-2}\) density light gain is gradually developed with increasing carrier density. At high density (i.e., when density is equal \(9 \times 10^{12}\) cm\(^{-2}\)) optical gain develops nearly in the spectral vicinity of the original optical gain at plasma density, which is equal \(7 \times 10^{12}\) cm\(^{-2}\).

The behavior light gain coefficient for two quantum well width and at given concentrations may be understood from Fig. 18(a,b), 19(c,d). From Fig. 18(a) one can see that overlap between the quantum confined electron and hole wave functions, related with the charge density distribution on the quantum well width, which are shown in Fig. 18(b), for
the wide quantum well is smaller than in the case for the narrow quantum well, and reduces stronger at decreasing carrier density.

The effective screening electric field distributions of the wide bandgap GaN/AlGaN quantum well systems, which are presented in Fig. 19(c) are similar to electric field in condenser.

As shown in Fig. 21, the situation is quite different in the 3.9 nm GaN/Al$_{0.3}$Ga$_{0.7}$N quantum well structure. Because of the weaker quantum confinement in this relatively wide quantum well, the piezoelectric field is able to significantly reduce the overlap between the quantum confined electron and hole wave function, that one can see from comparison researches similar to those, which is presented in Fig. 18,19. Consequently, the interband dipole matrix element or oscillator strength is substantially smaller than in the case for the narrow 2.6 nm quantum well. This intrinsic quantum confined Stark effect also significantly redshifts the gain maximum at plasma density $7 \times 10^{12}$ cm$^{-2}$ relative to the flat band situation. As the plasma density increases, the screening of the QCSE increases the electron-hole wave function overlap, and hence, the exciton oscillator strength. Simultaneously, there is a weakening of the piezoelectric field induced redshift, leading to to the net blueshift in gain maximum and absorption edge with increasing plasma density, as shown in Fig. 21.

To calculate density dependence of many-body Coulomb effects in absorption spectra of GaN quantum well we apply the same method developed by Koch et al. 56–58. Numerically solving the microscopic polarization equations we see that with increasing plasma density optical gain (i.e., negative absorption) develops in the spectral region of the original exciton resonance. With increasing free-carrier density the ionization continuum red shifts rapidly to long wavelength, while the 1s-exciton absorption line stays almost constant, due to the high degree of compensation between the weakening of the electron-hole binding energy and band-gap reduction like as was early found for GaAs$^7$. At high electron-hole concentration the electric-dipole momentum renormalization effects give rise to a large optical gains which are shown in Fig. 22,23. The maximum of Hartree-Fock gain spectrum is equal 29991 cm$^{-1}$ closes to wavelength of $\lambda = 339.1$ nm at the concentration $9 \times 10^{12}$ cm$^{-2}$. From Fig. 23, one can see, that Hartree-Fock spectrum is shifted long wavelength side relatively Hartree gain spectrum and a large Sommelfeld or Coulomb enhancement is present in quantum well. It is caused of the increasing of oscillator strength due to the electron-hole Coulomb attraction.

The calculation of exchange Hartree-Fock energy spectrum renormalization is accounted in motion equation for microscopic dipole due to electron-hole pair. For high concentration this value is available significant. Somewhat larger for electrons and less for holes. The total this value is reflected in Hartree-Fock gain shifting in comparison with Hartree spectrum, as shown in Fig. 23. It should be noted, that in gain spectrum is accounted not only Hartree-Fock correlations, but correlations higher order in development at Coulomb potential energy than Hartree-Fock. It achieve by summation of series in microscopical polarization equation at Coulomb energy in all order of perturbation theory. In detail microscopic polarization equation for dipole due to electron-hole pair for wurtzite quantum well will be considered in our next paper.

C. Conclusions

In summary, the self-consistant calculations of Schrödinger equations and Poisson equation of wide bandgap GaN/AlGaN quantum well systems predict interesting the quantum well width and charge density dependence of both the matrix elements for dipole optical interband transitions, and light gain spectrum. A blueshift with increasing plasma density in gain in relatively wide wells occurs as a consequence of the screening of the piezoelectric field induced quantum confined Stark effect. While structures with narrow well widths exhibit the usual dependent developing of the light gain maximum almost without shifting spectral region. It is found, that the matrix elements of optical transitions from the heavy hole band as well as light gain spectrum have the strict TE light polarizations. A red shifting Coulomb interacted carriers optical gain relatively of free density optical gain spectrum and a large Coulomb enhancement are found.

V. RASHBA SPIN SPLITTING IN ZINC-BLENDE GAN QUANTUM WELLS

Strain effects on the valence band spectra, the interband matrix elements, and the light gain spectrum in zinc-blende GaN quantum wells are studied. In the framework of the effective mass theory, the Schrödinger equation is solved for the valence bands with a $3 \times 3$ block Hamiltonian. The results are illustrated for the GaN/Al$_{0.19}$Ga$_{0.81}$N quantum well. It is found, 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. It is shown, that 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)].

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$^{30,145,146,171,172}$. A number of ultraviolet light-emitting diodes$^{31,173–177}$ and laser diodes$^{178–184}$ 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$^{185–187}$. 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: $\epsilon_{xx} = \epsilon_{yy} = x (a_{0}^{\text{AlN}} - a_{0}^{\text{GaN}})/a_{0}^{\text{AlGaN}} = -0.029x < 0$, when as $\epsilon_{xy} = \epsilon_{xz} = \epsilon_{yz} = 0$.$^{188}$ The longitudinal component of strain can be expressed as $\epsilon_{zz} = -2 (C_{12}/C_{11}) \epsilon_{xx}$, 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 thick film GaN.

To describe the emission or absorption processes the energies, as well as the wave functions of the lowest conduction subband and the valence subbands are calculated. The strain dependence of both the matrix elements for dipole optical interband transitions, and the light gain spectrum in zinc-blende GaN quantum wells are derived.

The point group of the zinc-blende structure are identical to the elements of the point group of a tetrahedron which is denoted by $T_d$. The space group of the zinc-blende structure is symmorphic and is denoted by $T_d^{269}$. The bonding between 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$^6$. 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$^6$.

The space group of the wurtzite structure is $C_{6h}$. The cohesive energy of the wurtzite structure is very close to that of the zinc-blende structure$^{69}$. For that reason, GaN can crystallize in both zinc-blende and wurtzite polytypes.

It is known$^{6,69,165,189}$, 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$^{189}$. Later, an derivation of the wurtzite Hamiltonian based the method of invariants with including the effects on the hole spectra has been proposed$^{6,190}$. 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$^{165,191}$. 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$^{187,165,191}$. Later approaches$^{87,165,191}$ are used in this work.

The paper is organized as follows. In Sec. II we introduce the known Hamiltonian of the valence band of both zinc-blende and wurtzite GaN structures. The wave functions of the conduction band and the valence band for an infinitely deep quantum well are presented. The momentum matrix elements, and the light gain coefficient are presented. In Sec. III the calculated original results of the strain dependence of the subband structures, the momentum matrix
Figure 24. (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.

elements, and the light gain spectrum are presented. Sec. IV summarizes the present studies.

A. Theory

It is known\textsuperscript{192}, that the optical material gain can be calculated from Fermi golden rule:

$$\alpha_0 = \frac{\pi e^2}{\varepsilon \sqrt{m_0 c^2}} \sum_{\sigma_z = \pm} \sum_{\sigma_z = \mp} \sum_{m,\alpha} \int k_t \, dk_t \int \frac{d\vec{p}}{2\pi} \left| e M^{\sigma_z,\sigma_z}_{m,\alpha}(k_t) \right|^2 \times \left( f^c_{m}(k_t) - f^v_{\sigma_z,\alpha}(k_t) \right) \delta(E_{cv,\sigma_z,m,\alpha}(k_t) - \hbar \omega),$$

(225)

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, $f^c_m$, $f^v_{\sigma_z,\alpha}$ are the Fermi-Dirac distributions for electrons in the conduction and valence bands, $e$ is a unit vector of vector potential of electromagnetic field, $E_{cv,\sigma_z,m,\alpha}(k_t)$ 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. The modal gain, which determines the threshold condition of a laser, is proportional to the material gain multiplied by the optical confinement factor $\Gamma$, which is proportional to the well width, and the number $a$ of quantum wells in the multiple quantum wells: $\alpha = \alpha_0 \Gamma a$. We take $\Gamma$, which is equal 0.01, $a$ is equal 1 in the calculations.

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. $M^{\sigma_z,\sigma_z}_{m,\alpha}(k_t) = \langle \Psi_{\sigma_z,\alpha,k_t}^{c} | \hat{\mathbf{p}} | \Psi_{m,k_t}^{v} \rangle$ is the momentum matrix elements for transitions between the conduction band state $\Psi_{m,k_t}^{c}(z)$ and the valence band state $\Psi_{\sigma_z,\alpha,k_t}^{v}(z)$, and $\hat{\mathbf{p}}$ 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 $m$th conduction subband
Figure 25. (Color online) GaN/AlGaN quantum well with the compressive biaxial strain $\epsilon_{xx} = -0.54\%$: (a) the valence subband structure; the momentum matrix elements for (b) the x- (or y-) polarization and (c) the z-polarization.

Figure 26. (Color online) GaN/AlGaN quantum well with the tensile biaxial strain $\epsilon_{xx} = 0.54\%$: (a) the valence subband structure; the momentum matrix elements for (b) the x- (or y-) polarization and (c) the z-polarization.
can be written as
\[ \Psi_{m,k}^{c \sigma_c}(r) = \frac{\epsilon^j k_z \rho_t}{\sqrt{A}} \chi_m(z)|S\rangle|\sigma_c\rangle, \]  
(226)
where \( A \) is the area of the quantum well in the \( xy \) plane, \( \rho_t \) is the two-dimensional vector in the \( xy \) plane, \( k_t = (k_x, k_y) \) is in-plane wave vector, and \( \chi_m(z) \) is the \( z \)-dependent part of the envelope function.

To symmetrize the p-like valence band, one can consider of the similarity between the p-like states and the atomic p wave functions\(^69\). It is known that p states are triple degenerate. We define three states with the orbital angular momentum \( l = 1 \) and the eigenvalues \( m_l \) of its \( z \) component:
\[ |1, \pm 1\rangle = (|X\rangle - i |Y\rangle)/\sqrt{2}, \]
\[ |1, 0\rangle = |Z\rangle, \]
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)\(^36\):
\[ |\Gamma_8(HH); \pm \frac{3}{2}\rangle = \frac{1}{\sqrt{2}} (|X\rangle - i |Y\rangle), \]
\[ |\Gamma_6(LH); \pm \frac{1}{2}\rangle = \frac{1}{\sqrt{3}} (|X\rangle - i |Y\rangle + \sqrt{2} |Z\rangle), \]
\[ |\Gamma_7(SH); \pm \frac{1}{2}\rangle = \frac{1}{\sqrt{3}} (\sqrt{2} |X\rangle - i |Y\rangle \mp |Z\rangle). \]
(227)
Defining of "\((l=1)\)-like" states in both zinc-blende and wurtzite GaN crystals is based on the Hamiltonian\(^6,163,189\):
\[ -H = \Lambda I + \Xi J_z^2 - \Delta_2 J_z \sigma_2 - \sqrt{2} \Delta_3 (J_+ \sigma_+ + J_- \sigma_-) + \Pi J_+^2 + \Pi^* J_-^2 + 2 \Sigma [J_z J_+] + 2 \Sigma^* [J_z J_-] \]
(228)
where
\[ \Lambda = \Delta_1 + \Delta_2 + A_1 k_z^2 + A_3 k_t^2 + D_1 \epsilon_{zz} + D_3 \epsilon_t, \]
\[ \Xi = -\Delta_1 + A_2 k_z^2 + A_4 k_t^2 + D_2 \epsilon_{zz} + D_4 \epsilon_t, \]
\[ \Pi = A_5 k_z^2 + D_5 \epsilon_z, \]
\[ \Sigma = A_6 k_z k_+ + D_6 \epsilon_{z-}, \]
\[ \Upsilon = \frac{i h^2 \Re k_-}{2 m_0}, \]
\[ k_\pm = k_x \pm i k_y, \quad k_\pm^2 = k_x^2 + k_y^2, \]
\[ J_\pm = \frac{1}{\sqrt{2}} (J_x \pm i J_y), \quad 2 [J_z J_\pm] = J_z J_\pm + J_\pm J_z, \]
\[ \sigma_\pm = \frac{1}{2} (\sigma_x \pm i \sigma_y), \]
\[ \epsilon_{\pm z} = \epsilon_{xz} \pm i \epsilon_{yz}, \quad \epsilon_\pm = \epsilon_{xx} - \epsilon_{yy} \pm 2 i \epsilon_{xy}, \]
\[ \epsilon_\ell = \epsilon_{xx} + \epsilon_{yy}. \]

The strain effects are included by addition of corresponding terms: \( k_i k_j \rightarrow \epsilon_{ij} \), with deformation parameters: \( D_1, D_2, \ldots, D_6 \) at the corresponding position of effective mass parameters: \( A_1, A_2, \ldots, A_6 \). Here \( m_0 \) is free electron mass, \( I \) is the unity matrix, \( J_x, J_y, \) and \( J_z \) are components of the angular momentum operator, \( \sigma_x, \sigma_y, \) and \( \sigma_z \) are Pauli matrices, \( \Delta_1 \equiv \Delta_{cr} \) is a splitting energy due to the hexagonal component of crystal field, \( \Delta_{so}^+ \equiv 3 \Delta_2 \) and \( \Delta_{so}^- \equiv 3 \Delta_3 \) are the spin-orbit splitting energy for \( z \) and perpendicular directions.

The term linear in the wave vector describes the circular loop of valence band maxima in crystals with wurtzite symmetry. For zinc-blende type materials, the term linear in the wave vector does not exist.

A transformation of the Hamiltonian written in the basis \( |1, m_1 \rangle |1/2, s \rangle \) to the basis of angular momenta \( 3/2 \) and \( 1/2 \) is performed with help of Eq. (227). By choosing a unitary transformation in manner similar to the cubic case:

\[ |1, \pm \rangle = \frac{1}{\sqrt{2}} |\pm i, \frac{3}{2}\rangle e^{-3 i \phi/2} \mp i |\frac{3}{2}, -\frac{3}{2}\rangle e^{3 i \phi/2}, \]
\[ |2, \pm \rangle = \frac{1}{\sqrt{2}} |\pm i, \frac{1}{2}\rangle e^{-i \phi/2} - |\frac{1}{2}, -\frac{1}{2}\rangle e^{i \phi/2}, \]
\[ |3, \pm \rangle = \frac{1}{\sqrt{2}} |\pm i, \frac{1}{2}\rangle e^{-i \phi/2} + |\frac{1}{2}, -\frac{1}{2}\rangle e^{i \phi/2}, \]

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

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

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

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

in the basis \( \{|1, \sigma_v\}, |2, \sigma_v\rangle, |3, \sigma_v\rangle \) where

\[ P = \frac{1}{3} \Delta_{cr} + \alpha_1 k_z^2 + \alpha_2 k_y^2 + d_1 \epsilon_{zz} + d_2 (\epsilon_{xx} + \epsilon_{yy}). \]
\[ Q = -\frac{1}{3} \Delta_{cr} - 2 \alpha_3 k_x^2 + \alpha_4 k_x^2 - 2 d_3 \epsilon_{zz} + d_4 (\epsilon_{xx} + \epsilon_{yy}), \]

\[ R = \sqrt{3} \alpha_5 k_x^2, \]

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

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

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

\[ \alpha_1 = A_1 + \frac{2}{7} A_2, \quad \alpha_2 = A_3 + \frac{3}{7} A_4, \quad \alpha_3 = -\frac{3}{7} A_2, \]

\[ \alpha_4 = \frac{1}{4} A_4, \quad \alpha_5 = -\frac{1}{4} A_5, \quad \alpha_6 = -\frac{3}{4} \sqrt{2} A_6, \]

\[ \Delta_{cr} = \Delta_1, \quad \Delta_{so} = 3 \Delta_2 = 3 \Delta_3. \]  

(232)

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

\[ d_1 = D_1 + \frac{2}{3} D_2, \quad d_2 = D_3 + \frac{2}{3} D_4, \]

\[ d_3 = -\frac{1}{6} D_2, \quad d_4 = \frac{1}{3} D_4. \]  

(233)

Parameters \(A_1 - A_6\) are related with a set of Luttinger-like parameters\(^{165}\):

\[-A_1 = \gamma_{1z} + 4 \gamma_{3z}, \quad -A_2 = \gamma_{1t} - 2 \gamma_{3t}, \quad A_3 = 6 \gamma_{3z} \]

\[-A_4 = 3 \gamma_{3t}, \quad A_5 = \gamma_{2t} + 2 \gamma_{3t}, \quad A_6 = \sqrt{2} (2 \gamma_{2z} + \gamma_{3z}). \]  

(234)

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

\[-D_1 = \delta_{1z} + 4 \delta_{3z}, \quad -D_2 = \delta_{1t} - 2 \delta_{3t}, \quad D_3 = 6 \delta_{3z} \]

\[-D_4 = 3 \delta_{3t}, \quad D_5 = \delta_{2t} + 2 \delta_{3t}, \quad D_6 = \sqrt{2} (2 \delta_{2z} + \delta_{3z}). \]  

(235)

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\(^{166}\):

\[ \gamma_{1z} = \gamma_{1t} \rightarrow \gamma_1, \quad \gamma_{2z} = \gamma_{2t} \rightarrow \gamma_2, \quad \gamma_{3z} = \gamma_{3t} \rightarrow \gamma_3, \]  

(236)

\[ \delta_{1z} = \delta_{1t} \rightarrow -a, \quad \delta_{2z} = \delta_{2t} \rightarrow -b/2, \]

\[ \delta_{3z} = \delta_{3t} \rightarrow -d/2\sqrt{3}. \]  

(237)

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\(^{69}\). 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:

\[ |\alpha \sigma_v, k_t\rangle = \begin{pmatrix} \phi^{(1)}_\alpha (z, k_t) \\ \phi^{(2)}_\alpha (z, k_t) \\ \phi^{(3)}_\alpha (z, k_t) \end{pmatrix} |1, \sigma_v\rangle, \]

(238)

\[ \phi^{(j)}_\alpha = \sum_{i=1}^a \chi^{(j)}_{k_t} (i, \alpha) \chi_i (z), \]

(239)

and \(j = 1, 2, 3\). The Bloch vector of \(\alpha\)-type hole with spin \(\sigma_v = \pm\) and momentum \(k_t\) is specified by its three
coordinates \([V_{k_0}^{(1)}[n, \alpha], V_{k_1}^{(2)}[n, \alpha], V_{k_2}^{(3)}[n, \alpha]]\) in the basis \([1, \sigma_v], [2, \sigma_v], [3, \sigma_v]\). 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

\[
\chi_n(z) = \sqrt{\frac{2}{w}} \sin \left(\pi n \left(\frac{z}{w} + \frac{1}{2}\right)\right),
\]

where \(n\) is a natural number. The hole wave function can be written as

\[
\Psi^{\sigma_\pi}_{n, k_0}(r) = \frac{e^{ik_0 r}}{\sqrt{A}} |\alpha \sigma_\pi k_0\rangle.
\]

The valence subband structure \(E^\sigma_\alpha(k_i)\) can be determined by solving

\[
\sum_{j=1}^{3} (H_{ij}^\sigma_\alpha(k_z) = -i \frac{\partial}{\partial z} + \delta_{ij} E^\sigma_\alpha(k_i)) \phi^{(j)\sigma_\pi}(z, k_i) = 0,
\]

where \(i = 1, 2, 3\).

The only nonzero matrix elements between the basis functions exist\(^{36,165}\):

\[
\begin{align*}
\langle S|\hat{p}_z|1, 0 \rangle &= P_z, \\
\langle S|\hat{p}_z|1, -1 \rangle &= -\langle S|\hat{p}_z|1, 1 \rangle = \sqrt{2} P_z,
\end{align*}
\]

due to symmetry properties of the Bloch functions, where \(\hat{p}_x = \hat{p}_x \pm i \hat{p}_y\). Two momentum matrix elements constants can be defined as: \(P_{\perp} \equiv \langle S|\hat{p}_x|X\rangle\) and \(P_{\parallel} \equiv \langle S|\hat{p}_z|Z\rangle\).

The momentum-matrix elements for the \(x\) - (or \(y\) -) polarization (\(e \perp z\)) can be defined as\(^{194}\):

\[
|e_x M^\dagger_{m, \alpha}(k_i)^2 = \frac{[\langle S|\hat{p}_x|X\rangle]}{4} \times \left(\langle \chi_m |\phi^0_\alpha |\rangle^2 + \frac{1}{4} \langle \chi_m |\phi^2_\alpha |\rangle^2 + \frac{3}{2} \langle \chi_m |\phi^3_\alpha |\rangle^2 + \frac{\sqrt{3}}{2} \cos 2 \phi \langle \chi_m |\phi^1_\alpha |\rangle \langle \chi_m |\phi^2_\alpha |\rangle + \sqrt{\frac{3}{2}} \cos 2 \phi \langle \chi_m |\phi^1_\alpha |\rangle \langle \chi_m |\phi^3_\alpha |\rangle \right).
\]

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

\[
|e_z M^\dagger_{m, \alpha}(k_i)^2 = \frac{[\langle S|\hat{p}_z|Z\rangle]^2}{4} \left(\langle \chi_m |\phi^0_\alpha |\rangle^2 + \frac{1}{2} \langle \chi_m |\phi^3_\alpha |\rangle^2 + \sqrt{2} \langle \chi_m |\phi^3_\alpha |\rangle \langle \chi_m |\phi^3_\alpha |\rangle \right).
\]

It is known\(^{165}\) that the values of constants \(|P_{\perp, \parallel}|^2\) can be found from kp theory

\[
\frac{m_0}{m_{\perp, \parallel}^{(c)}} = 1 + \frac{2}{m_0} \sum_{j \neq c} \frac{[\langle \hat{p}_z, j \rangle]}{E_j - E_0^0} E_j^0
\]

and from experimentally measured conduction band effective mass \(m_{\perp, \parallel}^{(c)}\) can be estimated

\[
\frac{2 |P_{\perp, \parallel}|^2}{m_0} \simeq E_j \left(\frac{m_0}{m_{\perp, \parallel}^{(c)}} - 1\right)
\]

Here we use the effective-mass parameters, spin-orbit splitting energy, and deformation potential parameters as in papers\(^{165,194,195}\).

**B. Results and discussions**

We consider the pseudomorphically strained zinc-blende GaN/Al\(_{0.19}\)Ga\(_{0.81}\)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 \( k_t = (k_x, k_y) \), which lies in plain of the quantum well, are presented in Figs. 24-26. 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. 24, we show the valence-band structure and the k-dependence of the matrix elements. Fig. 24a 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\(^{196} \). This implies removing of the degeneracy of the \( \Gamma_8 \) state. It is shown in the Fig. 24a.

In Fig. 25, 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: \( \epsilon_{xx} = -0.0054, \epsilon_{zz} = 0.0063 \). This strain is consistent with the aluminum content 19%. In Fig. 25a 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\(^{197} \).

We consider optical transitions between the initial and final states such as: with angular momentum \( J = 3/2 \) and the magnetic quantum numbers \( m_J = \pm 3/2, m_J = \pm 1/2 \) as well as with \( J = 1/2, m_J = \pm 1/2 \) of the valence band and with \( J = 1/2, m_J = \pm 1/2 \) of the conduction band. Transitions from the valence band states \( m_J = \pm 1/2 \) 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 \( m_J = \pm 3/2 \) obey selection rules \( \Delta m = \pm 1 \), therefore they have only the x (or y) polarization\(^{29} \).

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. 24, 25 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 \( \epsilon_{xx} = -0.0054 \). 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\(^{6,159,198} \) 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. 26 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: \( \epsilon_{xx} = 0.0054, \epsilon_{zz} = -0.0063 \). In Fig. 26a 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 splitting width due to an upward shift of the light valence band to the top of heavy hole band. The former leads to can see, that the tensile strain causes both the strong transformation of the hole effective mass and a decrease of the

In zinc-blende GaN the states of the light hole band are composed of the \( |X \pm iY\rangle \) characters as well as the \( |Z\rangle \) character. Comparing Figs. 24, 26 show an increase of presence of the \( |Z\rangle \) state in the light hole band as one moves from the unstrained thin film to the strained heterostructure, in which \( \epsilon_{xx} = 0.0054 \). There is more the \( |Z\rangle \) state in the light hole band in the strained heterostructure, than in the thin film. Therefore in the strained quantum well with \( \epsilon_{xx} > 0.0054 \), the states of the highest-lying light hole band are almost composed of the \( |Z\rangle \) 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.
In Fig. 27, we show the energy-dependence of the light gain coefficient of the quantum well with the carrier concentration $5 \times 10^{12} \text{cm}^{-2}$ at the temperature 4.4K for the such light polarization, optical transitions in which, are allowed by the selection rules and the calculated matrix elements. As soon as we obtain the interband population inversion, the light become amplified. At high carrier densities, the stimulated optical transitions give rise to the large optical gain. It is shown, that under the compressive strain, the shift of the valence and conduction bands leads to a blue shift of the gain spectra, with respect of the band-edge of unstrained quantum well.

It is found, that the effective mass is drastically changed under the tensile strain. This leads to change of sign and polarization of the gain coefficient, as shown in Fig. 27. It can be explained of arising of the circular loop with radius $k_z \sim 0.7 \times \text{nm}^{-1}$ in valence band structure of zinc-blende GaN quantum well under the tensile strain. The extremum loop effects in the band structure of wurtzite symmetry, in which exists the linear term in wave vector, are known from papers. 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 wurtzite crystal structures each atom is surrounded by four nearest neighbors forming an ideal tetrahedron. The valence electrons of such crystal structure form hybridized $sp^3$ orbitals. This $sp^3$ 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, 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 $sp^3$ hybrids towards $sp^2$ and $p_z$ orbitals. The quantum mechanical problem of dehybridization $sp^3$ hybrids towards $sp^2$ and $p_z$ 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. 26c.

Our theoretical studies have well agreement with the experimental results.

C. 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 $3 \times 3$ 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 $\epsilon_{xx} = -0.54\%$, the matrix elements for transitions from the first hole band have the strict $x$ (or $y$) light polarization, when as with the tensile strain $\epsilon_{xx} = 0.54\%$, 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 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 of valence band maxima. It is shown, that laser effect is suppressed in GaN quantum well with the tensile strain $\epsilon_{xx} = 0.54\%$, while at $\epsilon_{xx} = -0.54\%$ 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 effects in wurtzite crystals were studied, suppressing of laser effect was not indicated in publications. 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. It is found that the internal strain effects play the significant role on the optical properties in the quantum well heterostructures.
VI. LIGHT STIMULATED INSTABILITY OF SURFACE PLASMON POLARITONS AT GRAPHENE/METAL INTERFACE

Optical ground states of two surface plasmon polaritons in graphene in the vicinity of Dirac point phototransitions are found if magnetic field is applied. We found the analytical solutions of Maxwell equations in Majorana form for two coupled surface plasmon polaritons in Dirac point of honeycomb lattice. Surface plasmon polariton pair instability for supercritical scaling of honeycomb lattice is predicted via resonant states with complex number energies. It signifies the existing of the tachyon solutions in Maxwell equations in Majorana form for definition of optical ground states of two surface plasmon polaritons of honeycomb lattice. In the paper we derive some attractive expressions involving such higher transcendental functions as confluent hypergeometric functions and hypergeometric functions for the inner product space with respect to the weighted inner product \( \int_{0}^{\infty} e^{-\lambda z} z^{-1} F(\alpha, \gamma, k z) F(\alpha', \gamma', k' z) dz \).

A. Stimulated emission coefficient for the intrinsic graphene in magnetic field

Consider the intrinsic graphene under the applied magnetic field perpendicularly to the graphene plane. Weyl-Wallace Hamiltonian in the Landau gauge for the vector potential \( A = B (0, x, 0) \) of a curl field can find in the form:

\[
\hat{H} = v_F \begin{bmatrix}
0 & p_x + i p_y + \frac{ieB}{c} x \\
p_x + i p_y + \frac{ieB}{c} x & 0
\end{bmatrix}.
\]  

(248)

Consider a Dirac fermions in an electric field \( E_\omega e^{-i\omega t} + c.c \). The Hamiltonian of an intrinsic graphene can be found as following

\[
\hat{h} = v_F (\hat{\sigma} p) \text{ with the Pauli matrices pseudospin } \hat{\sigma} \text{ and the perturbation operator } i e v_F \omega (\hat{\sigma} E_\omega) e^{-i\omega t} + c.c.
\]

The phototransition probability \((l'p' \rightarrow lp)\) can express by the Fermi golden rule:

\[
W_{lp' \rightarrow l'p'} = \frac{2\pi}{\hbar} \sum_{l} \int \frac{\delta(E_{lp'} - E_{l'p'} - \hbar \omega)}{\delta(\epsilon_{lp'} - \epsilon_{l'p'} - \hbar \omega)} |\langle lp | \hat{\sigma} E_\omega | l'p' \rangle|^2 \omega d\omega.
\]

(249)

where \( l, l' = \pm 1 \).

In the case if the light wave length is larger than cyclotron orbit radius then the stimulated emission coefficient can express as follows \(204,205 \):

\[
R = \frac{\epsilon^2 v_F^2}{\pi c} \int \frac{\delta(E_{lp'} - E_{l'p'} - \hbar \omega)}{\delta(\epsilon_{lp'} - \epsilon_{l'p'} - \hbar \omega)} \omega d\omega.
\]

(250)

Dirac equation:

\[
v_F \begin{bmatrix}
0 & p_x + i p_y + \frac{ieB}{c} x \\
p_x + i p_y + \frac{ieB}{c} x & 0
\end{bmatrix} \begin{bmatrix}
\varphi_1 \\
\varphi_2
\end{bmatrix} = E \begin{bmatrix}
\varphi_1 \\
\varphi_2
\end{bmatrix},
\]

(251)

presents the homogenous system the solutions of which exist if system determinant is not equal zero. From this condition can conclude about Landau quantization of energy spectrum \( E^2 = \frac{2h^2 v_F^2}{l_B^2} n \). The length scale if the magnetic field is applied \( l_B = \sqrt{\frac{\epsilon B}{\hbar^2}} \), allows to find the energy spectrum in the form \(100 \): \( E = sgn(n) \alpha \sqrt{n} \), where \( n \) is a number of natural number set, \( \alpha = \frac{\sqrt{2\hbar v_F}}{l_B} \).

The eigenvalues of energy \( E^2 \) correspond the wave vector

\[
\Psi_{n \neq 0} = \frac{1}{\sqrt{2}} \begin{bmatrix}
-sgn(n) i \psi_{|n| - 1} \\
\psi_{|n|}
\end{bmatrix},
\]

(252)
Figure 28. (Color online) Single-particle spectrum of graphene for massless Dirac fermions (Majorana fermions) for wave vectors in a range $k_x = -2.318..2.318$ and $k_y = -2.318..2.318$ in a units of $1/A$.

$$\Psi_{n=0} = \frac{1}{\sqrt{2}} \left\| \begin{array}{c} 0 \\ \psi_0 \end{array} \right\|,$$  

(253)

where $\psi_n = e^{-\xi^2/2}H_n(\xi)$, $H_n(\xi)$-Chebyshev-Hermite polynomials, $\xi = s^{-1} \tilde{x}$, $\tilde{x} = x + x_0$, $x_0 = s^2 k_y$, $s^2 = \frac{eh}{c^2}$, $s \equiv l_B$, $\int_{-\infty}^{+\infty} H_n(\xi) H_m(\xi) \exp^{-\xi^2} d\xi = 2^n n! \sqrt{\pi} \delta_{nm}$.

Since

$$|(\Psi_n | \hat{\sigma}_{x,y} | \Psi_{n+1})|^2 = \frac{1}{4},$$  

(254)

then in graphene the current matrix elements are allowed for the stimulated emission coefficients derived by in the article 206.

$$R_{n+1 \rightarrow n} = \frac{\epsilon^2 v_F^2 E_0^2 \omega_c}{(n = 0)}$$  

$$R_{n+1 \rightarrow n} = \frac{\epsilon^2 v_F^2 E_0^2 \omega_c}{(n \neq 0)}.$$  

(255)

In the article 206 was estimated the stimulated emission coefficient. The stimulated emission coefficient for graphene in a weak magnetic fields are shown to be found $10^7 e^{-1}$, as well as for GaAs $6 \times 10^4 e^{-1}$. Hence the graphene can be of base for the quantum generator functioning. The amplified by the graphene quantum generator an electromagnetic waves can be narrowed at graphene/metal interface in result of light and plasma metal oscillations interactions. Hence can be derived the surface plasmon polaritons (SPPs) on a exit of waveguides.

B. Some mathematical expressions involving confluent hypergeometric functions and hypergeometric functions

The weighted inner product of confluent hypergeometric functions are given by

$$J = \int_0^\infty e^{-\lambda z} z^\gamma F(\alpha, \gamma, kz) F(\alpha', \gamma, k'z) dz,$$  

(256)

where

$$F(\alpha', \gamma, k'z) = -\frac{1}{2\pi i} \frac{\Gamma(1 - \alpha') \Gamma(\gamma)}{(\Gamma(1 - \alpha') - \Gamma(\gamma))} \int e^{tk'(-t)^{\alpha'-1}(1 - t)^{\gamma - \alpha' - 1}} dt.$$  

(257)

Consider the integral
\[ J_{\nu} = \int_{0}^{\infty} e^{-\lambda z \nu - 1} [F(-n, \gamma, k z)]^2 dz, \] (258)

where

\[ F(-n, \gamma, k z) = -\frac{1}{2\pi i} \frac{\Gamma(1+n)\Gamma(\gamma)}{\Gamma(\gamma+n)} \oint e^{tkz}(-t)^{-n-1}(1-t)^{\gamma+n-1} dt. \] (259)

Substituting (259) in (258) we found the integral in the form

\[ J_{\nu} = -\int_{0}^{\infty} e^{-\lambda z \nu - 1} \frac{1}{2\pi i} \frac{\Gamma(1+n)\Gamma(\gamma)}{\Gamma(\gamma+n)} \oint e^{tkz}(-t)^{-n-1}(1-t)^{\gamma+n-1} dt dz \times \left( -\frac{1}{2\pi i} \frac{\Gamma(1+n)\Gamma(\gamma)}{\Gamma(\gamma+n)} \oint e^{tkz}(-t')^{-n-1}(1-t'+tk)^{-\nu} dt' \right). \] (260)

Since

\[ \int_{0}^{\infty} e^{-\lambda z} e^{tkz} e^t \nu - 1 dz = (\lambda - tk - t'k)^{-\nu} \Gamma(\nu), \] (261)

then the Eq. (260) one can be rewritten in the form

\[ J = \left( -\frac{1}{2\pi i} \right)^2 \frac{\Gamma(1+n)\Gamma(\gamma)\Gamma(\nu)}{\Gamma(\gamma+n)} \oint e^{tkz}(-t)^{-n-1}(1-t)^{\gamma+n-1} dt \times \oint (-t')^{-n-1}(1-t')^{\gamma+n-1}(\lambda - tk - t'k)^{-\nu} dt'. \] (262)

If

\[ F(\alpha, \beta, \gamma, z) = -\frac{1}{2\pi i} \frac{\Gamma(1-n)\Gamma(\gamma)}{\Gamma(\gamma+n)} \oint (-t)^{-n-1}(1-t)^{\gamma+n-1} dt, \] (263)

\[ J = \left( -\frac{1}{2\pi i} \right)^2 \frac{\Gamma(1+n)\Gamma(\gamma)\Gamma(\nu)}{\Gamma(\gamma+n)} \oint e^{tkz}(-t)^{-n-1}(1-t)^{\gamma+n-1} dt \times \oint (-t')^{-n-1}(1-t')^{\gamma+n-1}(\lambda - tk - t'k)^{-\nu} dt', \] (264)

where

\[ F(-n, \nu, \gamma, \frac{k}{\lambda - tk}) = -\frac{1}{2\pi i} \frac{\Gamma(1+n)\Gamma(\gamma)}{\Gamma(\gamma+n)} \oint (-t')^{-n-1}(1-t')^{\gamma+n-1}(1-t') \frac{k}{\lambda - tk}^{-\nu} dt', \] (265)

then the integral given by formula of (264) we seek in the form

\[ J = \left( -\frac{1}{2\pi i} \right)^2 \frac{\Gamma(1+n)\Gamma(\gamma)\Gamma(\nu)}{\Gamma(\gamma+n)} \times \oint (-t)^{-n-1}(1-t)^{\gamma+n-1} dt (\lambda - tk)^{-\nu} F(-n, \nu, \gamma, \frac{k}{\lambda - tk}), \] (266)

where

\[ F(-n, \nu, \gamma, \frac{k}{\lambda - tk}) = \left( \frac{1}{\gamma(\gamma+1)\ldots(\gamma+n-1)} \right) \left( \frac{k}{\lambda - tk} \right)^{1-\nu} (1 - \frac{k}{\lambda - tk})^n \frac{d^n}{d(\frac{k}{\lambda - tk})^n} \left( (\frac{k}{\lambda - tk})^{\nu+n-1} (1 - \frac{k}{\lambda - tk})^0 \right). \] (267)

Since

\[ \frac{d^n}{dx^n} x^{\nu-1+n} = (\nu - 1 + n)! x^{\nu-1}, \] (268)

then
\[ F(-n, \nu, \gamma, \frac{k}{\lambda - tk}) = \frac{(\nu - 1 + n)!}{\gamma + 1 - 1} \left( 1 - \frac{k}{\lambda - tk} \right)^n. \]  

(269)

The solution of the integral given by formula of (270)

\[ J = -\frac{1}{2\pi i} \frac{\Gamma(1+n)\Gamma(\nu)}{\Gamma(\gamma + n)} \frac{(\nu - 1 + n)!}{\gamma + 1 - 1} \int \frac{-n-1}{(1-t)^{\gamma + n-1}}(\lambda - tk)^{-\nu - n}(\lambda - tk - k)^n dt = \]  

(270)

may be found by substitutions

\[ t \rightarrow \frac{\lambda t}{k t - \lambda + k}, \]  

(271)

\[ dt \rightarrow \frac{\lambda (k t - \lambda + k) + \lambda t k}{(k t - \lambda + k)^2} dt, \]  

(272)

of the following expression

\[ J = -\frac{1}{2\pi i} \frac{\Gamma(1+n)\Gamma(\nu)}{\Gamma(\gamma + n)} \frac{(\nu - 1 + n)!}{\gamma + 1 - 1} \int \frac{-n-1}{(1-t)^{\gamma + n-1}} \left( \frac{\lambda (\lambda - k)}{k t - \lambda + k} \right)^n \left( \frac{\lambda}{k t - \lambda + k} \right) dt + \frac{\lambda k}{(k t - \lambda + k)^2} dt \]  

(273)

after the similar algebraic transformations we find the solution of sought for integral as follows

\[ J = -\frac{1}{2\pi i} \frac{\Gamma(1+n)\Gamma(\nu)}{\Gamma(\gamma + n)} \frac{(\nu - 1 + n)!}{\gamma + 1 - 1} \int \frac{-n-1}{(1-t)^{\gamma + n-1}} \left( \frac{\lambda (\lambda - k)}{k t - \lambda + k} \right)^n \left( \frac{\lambda}{k t - \lambda + k} \right) dt + \frac{\lambda k}{(k t - \lambda + k)^2} dt \]  

(274)

After the similar algebraic transformations one can find

\[ J = \int_0^\infty e^{-\lambda z} z^{\gamma - 1} F(-n, \gamma, k z) F(a', \gamma, k' z) d z, \]  

(275)

\[ F(a', \gamma, k' z) = -\frac{1}{2\pi i} \frac{\Gamma(1+a')\Gamma(\gamma)}{\Gamma(\gamma - a')} \int e^{ztk'}(-t)^{a' - 1}(1 - t)^{\gamma - a' - 1} dt, \]  

(276)

\[ F(-n, \gamma, k z) = -\frac{1}{2\pi i} \frac{\Gamma(1+n)\Gamma(\gamma)}{\Gamma(\gamma + n)} \int e^{ztk}(-t)^{-n-1}(1 - t)^{\gamma + n-1} dt', \]  

(277)

\[ J = \int_0^\infty e^{-\lambda z} z^{\gamma - 1} \left( \frac{1}{2\pi i} \frac{\Gamma(1+a')\Gamma(\gamma)}{\Gamma(\gamma - a')} \int e^{ztk'}(-t)^{a' - 1}(1 - t)^{\gamma - a' - 1} dt \right) \times \]  

(278)

\[ \times \left( -\frac{1}{2\pi i} \frac{\Gamma(1+n)\Gamma(\gamma)}{\Gamma(\gamma + n)} \int e^{ztk}(-t)^{-n-1}(1 - t)^{\gamma + n-1} dt' \right), \]  

\[ \int_0^\infty e^{-\lambda z} e^{ktk'} e^{ktk} z^{\gamma - 1} d z = (\lambda - tk' - t'k)^{-\gamma} \Gamma(\gamma), \]  

(279)
\[
J = \left( -\frac{1}{2\pi} \right)^2 \frac{\Gamma(1-\alpha')\Gamma(\gamma)}{\Gamma(\gamma-\alpha')} \frac{\Gamma(1+n)\Gamma(\gamma)}{\Gamma(\gamma+n)} \times \notag \]
\[
\int (-t)^{\alpha'-1}(1-t)^{\gamma-\alpha'-1} dt \int (-t')^{-n-1}(1-t')^{\gamma+n-1}(\lambda - t k' - t' k)^{-\gamma} dt', \tag{280}
\]
\[
F(\alpha, \beta, \gamma, z) = -\frac{1}{2\pi} \frac{\Gamma(1-\alpha)\Gamma(\gamma)}{\Gamma(\gamma-\alpha)} \int (-t)^{\alpha-1}(1-t)^{\gamma-\alpha-1}(1-tz)^{-\beta} dt, \tag{281}
\]
\[
J = \left( -\frac{1}{2\pi} \right)^2 \frac{\Gamma(1-\alpha')\Gamma(\gamma)}{\Gamma(\gamma-\alpha')} \frac{\Gamma(1+n)\Gamma(\gamma)}{\Gamma(\gamma+n)} \times \notag \]
\[
\int (-t)^{\alpha'-1}(1-t)^{\gamma-\alpha'-1} dt \int (-t')^{-n-1}(1-t')^{\gamma+n-1}(\lambda - t k)\frac{k}{\lambda - tk'}^{-\gamma} dt', \tag{282}
\]
\[
F(-n, \gamma, \frac{k}{\lambda - tk'}) = -\frac{1}{2\pi} \frac{\Gamma(1+n)\Gamma(\gamma)}{\Gamma(\gamma+n)} \int (-t')^{-n-1}(1-t')^{\gamma+n-1}(\lambda - t k')\frac{k}{\lambda - tk'}^{-\gamma} dt', \tag{283}
\]
\[
J = \left( -\frac{1}{2\pi} \right)^2 \frac{\Gamma(1-\alpha')\Gamma(\gamma)}{\Gamma(\gamma-\alpha')} \frac{\Gamma(1+n)\Gamma(\gamma)}{\Gamma(\gamma+n)} \times \notag \]
\[
\int (-t)^{\alpha'-1}(1-t)^{\gamma-\alpha'-1} dt(\lambda - tk')^{-\gamma} F(-n, \gamma, \frac{k}{\lambda - tk'}), \tag{284}
\]
\[
F(-n, \gamma, \frac{k}{\lambda - tk'}) = \frac{1}{\gamma(\gamma+1)...(\gamma+n-1)} \frac{k}{\lambda - tk'}^{1-n} \frac{d^n}{dx^n} \left[ \left( \frac{k}{\lambda - tk'} \right)^{\gamma+n-1} \left( 1 - \frac{k}{\lambda - tk'} \right)^0 \right], \tag{285}
\]
\[
\frac{d^n}{dx^n} x^{\gamma+1+n} = (\gamma + n)！x^{\gamma-1}, \tag{286}
\]
\[
F(-n, \gamma, \frac{k}{\lambda - tk'}) = \frac{\gamma(\gamma+1)...(\gamma+n-1)}{\gamma(\gamma+1)...(\gamma+n-1)} \frac{k}{\lambda - tk'}^{1-n}, \tag{287}
\]
\[
J = -\frac{1}{2\pi} \frac{\Gamma(1-\alpha')\Gamma(\gamma)}{\Gamma(\gamma-\alpha')} \times \notag \]
\[
\int (-t)^{\alpha'-1}(1-t)^{\gamma-\alpha'-1}(\lambda - tk')^{-\gamma-n}(\lambda - tk')\frac{\gamma-n}{\lambda - tk'} dt = \tag{288}
\]
\[
\int (-t)^{\alpha'-1}(1-t)^{\gamma-\alpha'-1}(\lambda - tk')^{-\gamma-n}(\lambda - tk')\frac{\gamma-n}{\lambda - tk'} dt.
\]

The solution of the sought for integral one can find by replacements
\[
t \longrightarrow \frac{\lambda t}{k' t - \lambda + k}, \tag{289}
\]
\[
dt \longrightarrow \frac{\lambda k' t^2 - 2\lambda k t + \lambda^2}{(k' t - \lambda + k)^2} dt, \tag{290}
\]
in the following form after the algebraic transformations
\[
J = \left( -\frac{1}{2\pi} \right)^2 \frac{\Gamma(1-\alpha')\Gamma(\gamma)}{\Gamma(\gamma-\alpha')} \int (-t)^{\alpha'-1}(1-t)^{\gamma-\alpha'-1}(\lambda - k t + \lambda k')^{-\gamma-n}(\lambda - k t + \lambda k')^{\gamma-n} dt + \frac{\lambda k'}{(k' t - \lambda + k)^2} dt, \tag{291}
\]
The solution of the sought for integral one can be found as well as by the following replacements

After the similar algebraic transformations we can find the solution of sought for integral

where

We find the solution of sought for integral as follows

Let us consider the integral

where

After the similar algebraic transformations we can find the solution of sought for integral

and

Therefore

Finally

The solution of the sought for integral one can be found as well as by the following replacements

and

and

Therefore
\[
F(\alpha, \beta, \gamma, z) = -\frac{1}{2\pi i} \frac{\Gamma(1-\alpha)\Gamma(\gamma)}{\Gamma(1-\alpha)\Gamma(\gamma)} \int (-t)^{\alpha-1} (1-t)^{\gamma-\alpha-1} (1-tz)^{-\beta} dt,
\]

\[J_{\nu}^{p}(\alpha, \alpha') = (-\frac{1}{2\pi i})^2 \frac{\Gamma(1-\alpha)\Gamma(\gamma)\Gamma(1-\alpha')\Gamma(\gamma-p)\Gamma(\nu+s)}{\Gamma(1-\alpha)\Gamma(\gamma-\alpha')\Gamma(1-\nu-p)\Gamma(1-\gamma-\nu)} \int (-t)^{\alpha-1} (1-t)^{\gamma-\alpha-1} dt \times \int (-t')^{\alpha'-1} (1-t')^{\gamma-p-\alpha'-1} dt' \frac{(k' t - tk)}{(k' t + tk)} \nu-s, \]

\[F(\alpha', \nu + s, \gamma - p, \frac{k'}{x - tk}) = -\frac{1}{2\pi i} \frac{\Gamma(1-\alpha')\Gamma(\gamma-p)}{\Gamma(1-\alpha')\Gamma(\gamma-p)} \int (-t')^{\alpha'-1} (1-t')^{\gamma-p-\alpha'-1} (1 - \frac{t'k'}{x - tk})^{-\nu-s} dt', \]

\[J_{\nu}^{p}(\alpha', \alpha') = (-\frac{1}{2\pi i})^2 \frac{\Gamma(1-\alpha')\Gamma(\gamma)\Gamma(\nu+s)}{\Gamma(1-\alpha')\Gamma(\gamma-\alpha')\Gamma(1-\nu-s)} \int (-t)^{\alpha-1} (1-t)^{\gamma-\alpha-1} dt \times \frac{(k+k')}{2} - tk \nu-s F(\alpha', \nu + s, \gamma - p, \frac{k+k'}{2} - tk), \]

\[F(-n, \nu + s, \gamma - p, \frac{k'}{x - tk}) = \frac{1}{\Gamma(\gamma+1)} \frac{\Gamma(\gamma+n-k)}{\Gamma(\gamma+n-k)} \int \frac{d^n}{(k' t - tk)^n} \left( \frac{k'}{x - tk} \right)^{-\nu-s-\gamma+p} = \sum_{k=1}^{n} \frac{n!}{(n-k)!} (1-x)^{\alpha(k)} \gamma^{\alpha \beta(n-k)}, \]

\[x = \frac{k'}{x - tk}, \]

\[\beta = \gamma - p + n - 1, \]

\[\alpha = \nu + s - \gamma + p, \]

\[x^{\beta(n-k)} = (x^{\gamma-p+n-1})^{(n-k)} = (\gamma - p + n - 1)!x^{\gamma-p+k}, \]

\[((1-x)^{\nu+s-\gamma+p})^{(k)} = (\nu + s - \gamma + p)! (1-x)^{\nu+s-\gamma+p-k} (1)^{\nu+s-\gamma+p}, \]

\[\times \sum_{k=1}^{n} \frac{n!}{(n-k)!} (\gamma - p + n - 1)! (\nu + s - \gamma + p)! (1)^{\nu+s-\gamma+p-k} (1-x)^{\gamma+p-n-k}, \]

\[J_{\nu}^{p}(\alpha, -n) = (-\frac{1}{2\pi i})^2 \frac{\Gamma(1-\alpha)\Gamma(\gamma)\Gamma(\nu+s)}{\Gamma(1-\alpha)\Gamma(\gamma-n-1)\Gamma(1-\nu-s)} \int (-t)^{\alpha-1} (1-t)^{\gamma-\alpha-1} dt \times \sum_{k=1}^{n} (-1)^{\nu+s-\gamma+p} \frac{n!}{(n-k)!} (\gamma - p + n - 1)! (\nu + s - \gamma + p)! (\lambda - tk)^{-2\nu-2s+\gamma-p-n} (\lambda - tk - k')^{\nu+s-\gamma+p+n-1}, \]

\[t \rightarrow \frac{\lambda t}{\lambda + t - k}, \]
\[ dt \rightarrow \frac{\lambda}{k\tau + \lambda - k} dt + \frac{\lambda k t}{(k\tau + \lambda - k)^2} dt, \] (318)

if \( \alpha = -\nu - s + \gamma - p - n + l, \)

\begin{align*}
J^p_{\nu}(\alpha, -n) &= (-1) \cdot \frac{\Gamma(1 - \alpha)\Gamma(\gamma)}{\Gamma(\gamma + 1)} \Gamma(\nu + s) \frac{1}{(\gamma + n - 1)!} \times \\
& \times \left( -1 \right)^{\nu + s - \gamma + n} \frac{n!}{\Gamma(\gamma + n)} (\gamma - p + n - 1)! (\nu + s - \gamma + p) \times \\
& \times (\lambda^\gamma (\lambda - k')^{-\alpha} (\lambda - k)^{-\alpha} f (-t)^{\alpha - 1} (1 - t)^{\gamma - \alpha - 1} (1 - \frac{kk'}{(\lambda - k')(\lambda - k)})) - \alpha dt, \quad (319)
\end{align*}

\begin{align*}
J^p_{\nu}(\alpha, -n) &= (-1) \cdot \frac{\Gamma(1 - \alpha)\Gamma(\gamma)}{\Gamma(\gamma + 1)} \Gamma(\nu + s) \frac{1}{(\gamma + n + 1)!} \times \\
& \times \left( -1 \right)^{\nu + s - \gamma + n} \frac{n!}{\Gamma(\gamma + n - 1)} (\gamma - p + n - 1)! (\nu + s - \gamma + p) \times \\
& \times (\lambda^\gamma (\lambda - k')^{-\alpha} (\lambda - k)^{-\alpha} f (-t)^{\alpha - 1} (1 - t)^{\gamma - \alpha - 1} (1 - \frac{kk'}{(\lambda - k')(\lambda - k)})) - \alpha dt, \quad (320)
\end{align*}

Let us consider the integral

\[ J^p_{\gamma}(\alpha, \alpha') = \int_{0}^{\infty} e^{-\frac{k+k'}{z} - z} \gamma^{s} F(\alpha, s, \gamma + p, k'z) dz, \quad (321) \]

After the similar algebraic transformations we could find the solution of sought for integral

\begin{align*}
J^p_{\gamma}(\alpha, \alpha') &= (-1) \cdot \frac{\Gamma(1 - \alpha)\Gamma(\gamma)}{\Gamma(\gamma + 1)} \Gamma(\nu + s) \frac{1}{(\gamma + n - 1)!} \times \\
& \times \left( -1 \right)^{\nu + s - \gamma + n} \frac{n!}{\Gamma(\gamma + n)} (\gamma - p + n - 1)! (\nu + s - \gamma + p) \times \\
& \times (F(\alpha, \nu, s, \gamma, p, k') - \frac{kk'}{(\lambda - k')(\lambda - k)}\gamma^{s} F(\alpha + 1, \alpha, \gamma, \frac{kk'}{(\lambda - k')(\lambda - k)})), \quad (322)
\end{align*}

\begin{align*}
J^p_{\gamma}(\alpha, \alpha') &= (-1) \cdot \frac{\Gamma(1 - \alpha)\Gamma(\gamma)}{\Gamma(\gamma + 1)} \Gamma(\nu + s) \frac{1}{(\gamma + n - 1)!} \times \\
& \times \left( -1 \right)^{\nu + s - \gamma + n} \frac{n!}{\Gamma(\gamma + n)} (\gamma - p + n - 1)! (\nu + s - \gamma + p) \times \\
& \times (F(\alpha, \alpha, s, \gamma, p, k') - \frac{kk'}{(\lambda - k')(\lambda - k)}\gamma^{s} F(\alpha + 1, \alpha, \gamma, \frac{kk'}{(\lambda - k')(\lambda - k)})), \quad (323)
\end{align*}

\begin{align*}
(\gamma - \alpha - 1)J^p_{\gamma}(\alpha, \alpha') &= (\gamma - 1)J^p_{\gamma} + 1 p^{-1}(\alpha, \alpha') - \alpha J^p_{\gamma}(\alpha + 1, \alpha'), \quad (324)
\end{align*}

if \( \frac{k + k'}{2} = k, \)

\begin{align*}
J^0_{\gamma}(\alpha, \alpha') &= (-1) \cdot \frac{\Gamma(1 - \alpha)\Gamma(\gamma)}{\Gamma(\gamma + 1)} \Gamma(\nu + s) \frac{1}{(\gamma + n - 1)!} \times \\
& \times \left( -1 \right)^{\nu + s + \alpha - \gamma} \frac{n!}{\Gamma(\gamma + n)} (\gamma - p + n - 1)! (\nu + s + \alpha - \gamma) \times \\
& \times (F(\alpha, -s, \gamma, p, k') - \frac{k(k' + tk)}{k'}) \gamma^{s + \alpha} F(\alpha + 1, \gamma, -s, \gamma, \frac{k - k'}{k}), \quad (325)
\end{align*}

\begin{align*}
z = \frac{-k + k'}{2}, \quad (326)
\end{align*}

\begin{align*}
1 - z = \frac{k + k'}{2}, \quad (327)
\end{align*}

\begin{align*}
F(\alpha', -s, \gamma, z) &= \frac{z^{1 - \gamma}(1 - z)^{s + \alpha} d^s}{(\gamma + 1)! \ldots (\gamma + s) t} (z^{s + 1} (1 - z)^{\alpha - \gamma}), \quad (328)
\end{align*}
\[
\frac{d^n}{dz^n} z^{\gamma+s-1}(1-z)^{\alpha'-\gamma} = \sum_{i=1}^{n} \frac{s_i}{\Gamma(s-i)} ((1-z)^{\alpha'-\gamma}(z^{\gamma+s-1})^{(s-i)}),
\]
(329)

\[
(z^{\gamma+s-1})^{(s-i)} = (\gamma + s - 1)!z^{\gamma-1+i},
\]
(330)

\[
((1-z)^{\alpha'-\gamma})^{(i)} = (-1)^{\alpha'-\gamma}(\alpha' - \gamma)!((1-z)^{\alpha'-\gamma-i}(\gamma + s - 1)!z^{\gamma-1+i} =
\]
(331)

\[
F(\alpha', -s, \gamma, z) = \frac{z^{\gamma-\gamma}(1-z)^{\gamma+s-\alpha'}}{\gamma(\gamma+1)...(\gamma+s-s-1)} \sum_{i=1}^{s} \frac{s_i}{\Gamma(s-i)} ((1-z)^{\alpha'-\gamma}(\alpha' - \gamma)!(1-z)^{\alpha'-\gamma-i}(\gamma + s - 1)!z^{\gamma-1+i} =
\]
(332)

We find the solution of sought for integral as follows

\[
J_{s,0}^{\alpha}(\alpha', \alpha) = \frac{1}{2\pi i} k^{\gamma-s+\alpha'} \frac{\Gamma(1-\alpha)\Gamma(\gamma)}{\Gamma(1-\alpha)\Gamma(\gamma)} \frac{1}{(\gamma+2\alpha+1)!} (-1)^{\gamma-s+\alpha'} ((1-t)^{\gamma-s+\alpha'}(1-t)\Gamma(1-\alpha-t)\Gamma(\gamma-t)dt =
\]
(333)

\[
= \Gamma(\gamma + s)k^{\gamma-s+\alpha'}(k^2/k')^{\gamma-s+\alpha'} \frac{(-1)^{\gamma-s+\alpha'}(\gamma+s-1)!\Gamma(\gamma+s-1)!F(\alpha, \gamma + s - \alpha', \gamma, \frac{2k}{k+k'})}{\gamma(\gamma+1)...(\gamma+s-s-1)}. \]

C. Tachyonic solutions of Maxwell equations in Majorana form of two surface plasmon polaritons of graphene/metal interface

The graphene and graphene-like systems as well as the MX\(_2\) (M=Mo, W, X=S, Se)\(^1\) present a new state of matter of layered materials. The energy bands for graphite was found using "tight-binding" approximation by P.R. Wallace\(^2\). In the low-energy limit the single-particle spectrum is Dirac cone similarly to the light cone in relativistic mechanics, where the light speed is replaced by the Fermi velocity \(v_F\).

In the paper we present a theoretical investigation of excitonic states as well as their wave functions in gapped graphene and in a direct band MoS\(_2\). An integral form of the two-dimensional Schrödinger equation of Kepler problem in momentum space is solved exactly by projection the two-dimensional space of momentum on the three-dimensional sphere in the paper\(^6\).

The integral Schrödinger equation was analytically solved by the projection the three-dimensional momentum space onto the surface of a four-dimensional unit sphere by Fock in 1935\(^6\).

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 superconductivity.

If the exciton binding energy is greater than the flat band gap in narrow-gap semiconductor or semimetal then at sufficiently low temperature the insulator ground state is instable with respect to the exciton formation\(^1\)\(^1\)\(^5\)\(^1\)\(^8\). And excitons may be spontaneously created. In a system undergo a phase transition into an exciton insulator phase similarly to Bardeen-Cooper-Schrieffer (BCS) superconductor. In a single-layer graphene (SLG) and in a single-layer MoS\(_2\) the electron-hole pairing leads to the exciton insulator states\(^1\)\(^3\)\(^0\).

In the paper an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with complex dispersion is analytically solved. A complex dispersions lead to fundamental difference in exciton insulator states and their wave functions.

A crossing direct-gap like dispersion of single layer of graphene and single layer of MoS\(_2\) does not lead to the fundamental differences in the many-particle effects in comparison with wurtzite semiconductors\(^1\)\(^4\)\(^1\)\(^3\)\(^0\).

We analytically solve an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with electron-hole symmetry of reflection.

For graphene in vacuum the effective fine structure parameter \(\alpha_G = \frac{\varepsilon}{\varepsilon_{\text{vac}}^2} = 1.23\). For graphene in substrate \(\alpha_G = 0.77\), when the permittivity of graphene in substrate is estimated to be \(\varepsilon = 1.6\)\(^1\)\(^1\)\(^9\). It means the prominent Coulomb effects\(^1\)\(^2\)\(^0\).
It is known that the Coulomb interaction leads to the semimetal-exciton insulator transition, where gap is opened by electron-electron exchange interaction \(^{115,121-123}\). The perfect host combines a small gap and a large exciton binding energy \(^{115,118}\).

In graphene as well as in MoS\(_2\) the existing of bound pair states are still subject matter of researches \(^{112,124-127}\). It is known \(^{128}\) in the weak-coupling limit \(^{129}\), exciton condensation is a consequence of the Cooper instability of materials with electron-hole symmetry of reflection inside identical Fermi surface. The identical Fermi surfaces is a consequence of the particle-hole symmetry of Dirac equation. The room temperature superfluidity are shown to be calculated for bilayer graphene \(^{118,128}\).

The particle-hole symmetry of Dirac equation allows perfect pairing between electron Fermi sphere and hole Fermi sphere in the opposite layer and hence driving the Cooper instability. In the weak-coupling limit in graphene with the occupied conduction-band states and empty valence-band states inside identical Fermi surfaces in band structure, the exciton condensation is a consequence of the Cooper instability.

In the our paper \(^{207}\) the particle-hole pair instability for supercritical Coulomb potential is predicted via resonant states with complex number energies. It signifies the existing the tachyon solutions in Whittaker equations of which can be well known the Heisenberg equations in one-dimensional systems. These one-dimensional systems one can be carbon armchair ribbons in the vicinity of Dirac point in his spectrum within massless Dirac fermions (Majorana fermions).

1. Optical ground states of two surface plasmon polaritons in graphene in the vicinity of Dirac point phototransitions are found if magnetic field is applied

Surface plasmon polaritons (SPPs) can consider as Majorana bosons and described by the Maxwell equations in Majorana form in quantum electrodynamics (QED). It is known that a bosonic waves of SPPs propagate at the graphene/metal interface evanescently confined in the perpendicular direction.

We found the analytical solutions of Maxwell equations in Majorana form for two coupled surface plasmon polaritons in Dirac point of honeycomb lattice.

In the paper \(^{130}\) a theoretical study the both the quantized energies of excitonic states and their wave functions in gapped graphene and in monolayer of MoS\(_2\) is presented. An integral two-dimensional Schrödinger equation of the electron-hole pairing for a particles with electron-hole symmetry of reflection is analytically solved. The solutions of Schrödinger equation in momentum space in gapped graphene and in direct band monolayer of MoS\(_2\) by projection the two-dimensional space of momentum on the three-dimensional sphere are found. We analytically solve an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with electron-hole symmetry of reflection and with strong spin-orbit coupling. In monolayer of MoS\(_2\) as well as in single-layer graphene (SLG) the electron-hole pairing leads to the exciton insulator states. Calculating an integral two-dimensional Schrödinger equation of the electron-hole pairing for bilayer graphene, an exciton insulator states with a gap 3 meV are predicted. The particle-hole symmetry of Dirac equation of layered materials allows perfect pairing between electron Fermi sphere and hole Fermi sphere in the valence band and conduction band and hence driving the Cooper instability.

It is well known \(^{124}\) that the tachyonic instability can be considered as the fall into the center phenomenon. However in view of QED \(^{131,208}\) a ways of curing the instability in graphene are quite different from that in the case of the supercritical Coulomb charge. Since the coupling constant in freely standing graphene is larger than 1 the quasielectron in graphene has the supercritical Coulomb charge. In the opinion \(^{124}\) this leads to the production of an electron-hole pair via the coupling hole into the initial quasielectron forming a bound state but the emitted quasielectron has again a supercritical charge. Thus the process of creating pairs continues leading to the formation of exciton (chiral) condensate in the stable phase and as a result the quasiparticles acquire a gap. The exciton condensate formation resolves the problem of instability hence a gap generation should take place in a freely standing graphene making it an insulator.

In the paper \(^{132,133}\) a theoretical study the both the quantized energies of excitonic states and their wave functions in graphene is presented. An integral two-dimensional Schrödinger equation of the electron-hole pairing for a particles with electron-hole symmetry of reflection is exactly solved. The solutions of Schrödinger equation in momentum space in graphene by projection the two-dimensional space of momentum on the three-dimensional sphere are found exactly. We analytically solve an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with electron-hole symmetry of reflection. In single-layer graphene (SLG) the electron-hole pairing leads to the exciton insulator states. Quantized spectral series and light absorption rates of the excitonic states which distribute in valence cone are found exactly. If the electron and hole are separated, their energy is higher than if they are paired. The particle-hole symmetry of Dirac equation of layered materials allows perfect pairing between electron Fermi sphere and hole Fermi sphere in the valence cone and conduction cone and hence driving the Cooper instability.

We found the three acoustic branches and three optical branches which are are in close agreement with Ref. \(^{209}\). In
the framework our calculations one can conclude that in the K point the acoustic and optical branches have Dirac point similarly to the Dirac cone in graphene and light cone in relativistic physics, where the light velocity is substituted by the phonon velocity and describes by the Dirac equation.

For two surface plasmon polaritons one can find the Maxwell equations in Majorana (QED) form in the form:

$$\frac{d\Psi}{d\xi} = (j + \frac{1}{2}) \frac{\Psi}{\xi} + \frac{\xi}{2m^*} \Psi + \frac{E + \Delta}{\hbar v_{SPP}} \Phi = 0,$$

(334)
\[
\frac{d\Phi}{d\xi} + \left(j - \frac{1}{2}\right) \frac{\Phi}{\xi} - \frac{\xi}{2\Delta}\Psi - \frac{E - \Delta}{h v_{SPP}}\Psi = 0.
\] (335)

One can find the system of equations in a dimensionless values in the form:

\[
\rho \frac{d\psi}{d\rho} + \left(\frac{\rho}{2} - \frac{1}{4}\right) \psi + \frac{\rho}{2} \phi + j\phi = 0,
\] (336)

\[
\rho \frac{d\phi}{d\rho} - \left(\frac{\rho}{2} + \frac{1}{4}\right) \phi - \frac{\rho}{2} \phi + j\psi = 0,
\] (337)

where \(\Psi = \sqrt{\frac{m + \epsilon^2}{m - \epsilon^2}} (\psi - \phi), \Phi = \sqrt{\frac{m - \epsilon^2}{m + \epsilon^2}} (\psi + \phi), \epsilon = \frac{E}{h v_{SPP}}, m = \frac{\Delta}{h v_{SPP}}, u = \sqrt{m^2 - \epsilon^2}, \rho = \frac{2u}{l_B} \xi.\)

Substituting \(\phi\) from the first equation into the second one we find the equation for the \(\psi\) function

\[
\frac{d^2\psi}{d\rho^2} + \left(-\frac{1}{4} + \frac{1}{\rho} + \frac{1}{\rho^2} - \frac{\rho^2}{4}\right) \psi = 0,
\] (338)

of which is the well known Whittaker equation\(^{135-137}.\)

Its general solution is in the form of Whittaker functions

\[
\psi = C_1 W_{\kappa,\mu}(z) + C_2 M_{\kappa,\mu}(z),
\] (339)

where

\[
\kappa = \frac{1}{2}, \quad \mu = j.
\] (340)

For Whittaker functions can be written the following integral relation\(^{135-137}:\)

\[
\Gamma\left(\frac{1}{2} - \kappa + \mu\right) W_{\kappa,\mu}(z) = e^{-\frac{1}{4} z^2} z^{\mu + \frac{1}{2}} \times
\times \int_0^\infty e^{-t} t^{-\frac{1}{2} + \kappa + \mu} (1 + t)^{-\frac{1}{2} + \kappa + \mu} dt,
\] (341)

\[
W_{\kappa,\mu}(z) = e^{-z^2/2} z^\kappa \ {}_2F_0\left(\frac{1}{2} - \kappa + \mu, \frac{1}{2} - \kappa - \mu, -\frac{1}{2}\right),
\] (342)

\[
\Gamma\left(\frac{1}{2} - \kappa + \mu\right) \Gamma\left(\frac{1}{2} + \kappa + \mu\right) M_{\kappa,\mu}(z) = 2^{-2\mu} \Gamma(2\mu + 1) z^{\mu + \frac{1}{2}} \times
\times \int_{-1}^1 e^{t} t^{\frac{1}{2} - \kappa + \mu} (1 + t)^{-\frac{1}{2} - \kappa - \mu} dt.
\] (343)

In \(\xi > R\) range for supercritical scaling the solution of Eq. (338) we seek in the form

\[
f = C j W_{\kappa,\mu}(j \rho).
\] (344)

In \(\xi < R\) range for supercritical scaling the solution of Eqs. (336), (337) we seek as follows

\[
\psi = A_1 \xi J_{j+1/2}(\sqrt{\epsilon^2 - m^2} \xi),
\] (345)

\[
\phi = A_1 \text{sgn}(j) \sqrt{\frac{\epsilon^2 - m^2}{\epsilon^2 - m^2}} J_{j-1/2}(\sqrt{\epsilon^2 - m^2} \xi).
\] (346)
Under continuity conditions \(^36\) one can find on \(\xi = R\)

\[
\frac{W_{\epsilon,\nu}(j\rho)}{W_{\epsilon,\nu}(j\rho)} = \frac{k+1}{k-1},
\]

(347)

\[
k = \frac{1}{\text{sgn}(j)} \frac{1}{2\pi} \sqrt{\frac{e-m}{e+m}} j_0(\sqrt{e^2-m^2}\xi),
\]

(348)

where we have considered the states with the orbital quantum number \(j = \frac{1}{2}\) concerning of \(nS_{1/2}\) states i.e. the lowest-energy state belong to them.

\[
\epsilon = |e|e^{i\beta}.
\]

(349)

We analytically found the solution i.e. tachyon states within complex number quantized energies of the sought for equation (347) in the form:

\[
\ln(2|e|R) + i(\beta - \pi/2) \simeq 2\frac{j_0(\frac{1}{2})}{j_0(\frac{1}{2}) - j_1(\frac{1}{2})} + \psi(1) - \frac{1}{2}\psi(1 - \frac{1}{2}) - \frac{1}{\gamma} - \frac{\pi n}{\gamma},
\]

(350)

where we replace \(\gamma = i\nu\).

So we found the optical ground states of two SPPs in graphene in the vicinity of Dirac point if phototransitions are allowed when magnetic field is applied. We found the analytical solutions of Maxwell equations for two coupled SPPs in Dirac point of honeycomb lattice. SPPs pair instability for supercritical scaling of honeycomb lattice is predicted via resonant states with complex number energies. It signifies the existing of the tachyon solutions in Maxwell equations in Majorana form for definition of optical ground states of two SPPs of honeycomb lattice.

We found \(^207\) the resonant states for electron-hole pair in carbon nanoribbons in which the bound states dive into the lower continuum and determine by the complex number energies. Our results are in close agreement with Ref. \(^124\).

In the our paper \(^207\) the particle-hole pair instability for supercritical Coulomb potential is predicted via resonant states with complex number energies. It signifies the existing the tachyon solutions in Whittaker equations of which can be well known the Heisenberg equations in one-dimensional systems. These one-dimensional systems one can be carbon armchair ribbons in the vicinity of Dirac point in his spectrum within massless Dirac fermions (Majorana fermions).

### D. Conclusions and discussions

Fermi optical ground states of electron-hole pair in carbon nanoribbons \(^134\) in the vicinity of Dirac point were found in the articles \(^207\). We found the analytical solutions from equation of motion for polarization operators within Hartree-Fock approximation. Particle-hole pair instability for supercritical Coulomb potential is predicted via resonant states with complex number energies. It signifies the existing of the tachyon solutions in Whittaker equations of which can be well known the Heisenberg equations in one-dimensional systems.

The integral Schrödinger equation for a parabolic bands was analytically solved by the projection the three-dimensional momentum space onto the surface of a four-dimensional unit sphere by Fock in 1935 \(^62\). In integral form of the two-dimensional Schrödinger equation of Kepler problem in momentum space is solved exactly by the projection of the two-dimensional space of momentum on the three-dimensional sphere in the paper \(^61\).

In graphene the existing of bound pair states are still subject matter of researches \(^7\).

In the paper an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with complex dispersion is analytically solved. A complex dispersions lead to fundamental difference in exciton insulator states and their wave functions.

We analytically solve an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with electron-hole symmetry of reflection.

It is known that the Coulomb interaction leads to the semimetal-exciton insulator transition, where gap is opened by particle-particle exchange interaction \(^118\). The perfect host combines a small gap and a large exciton binding energy \(^118\).
We consider the pairing between oppositely charged particles in a material with "Mexican hat" shape band structure dispersion or in materials with giant Rashba spin splitting and in graphene. The Coulomb interaction leads to the electron-hole bound states scrutiny study of which acquire significant attention in explanations of high-temperature superconductivity.

It is known if the exciton binding energy is greater than the flat band gap in narrow-gap semiconductor or semimetal then at sufficiently low temperature the insulator ground state is unstable concerning to the exciton formation with follow up spontaneous production of excitons. In a system undergo a phase transition into an exciton insulator phase similarly to BCS superconductor. In a semiconductors with "Mexican hat" shape band structure dispersion as well as in graphene the electron-hole pairing leads to exciton insulator states.

The integral Schrödinger equation for a parabolic bands was analytically solved by the projection the three-dimensional momentum space onto the surface of a four-dimensional unit sphere by Fock in 1935.

In the paper an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with complex dispersion is analytically solved. A complex dispersion leads to fundamental difference in the energy of exciton insulator states and their wave functions.

We analytically solve an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with electron-hole symmetry of reflection.

It is known that the Coulomb interaction leads to the semimetal-exciton insulator transition, where gap is opened by electron-electron exchange interaction. The perfect host combines a small gap and a large exciton binding energy.

The particle-hole symmetry of Dirac equation of layered materials allows perfect pairing between electron Fermi sphere and hole Fermi sphere in the valence band and conduction band and hence driving the Cooper instability. In the weak-coupling limit in graphene with the occupied conduction-band states and empty valence-band states inside identical Fermi surfaces in band structure, the exciton condensation is a consequence of the Cooper instability.

In the paper a theoretical study the both the quantized energies of excitonic states and their wave functions in gapped graphene and in monolayer of MoS2 is presented. An integral two-dimensional Schrödinger equation of the electron-hole pairing for a particles with electron-hole symmetry of reflection is analytically solved. The solutions of Schrödinger equation in momentum space in gapped graphene and in the direct band monolayer of MoS2 by projection the two-dimensional space of momentum on the three-dimensional sphere are found. We analytically solve an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with electron-hole symmetry of reflection and with strong spin-orbit coupling. In monolayer of MoS2 as well as in single-layer graphene (SLG) the electron-hole pairing leads to the exciton insulator states. Calculating an integral two-dimensional Schrödinger equation of the electron-hole pairing for bilayer graphene, an exciton insulator states with a gap 3 meV are predicted. The particle-hole symmetry of Dirac equation of layered materials allows perfect pairing between electron Fermi sphere and hole Fermi sphere in the valence band and conduction band and hence driving the Cooper instability.

It is well known that the tachyonic instability can be considered as the fall into the center phenomenon. However in view of QED a ways of curing the instability in graphene are quite different from that in the case of the supercritical Coulomb center. Since the coupling constant in freely standing graphene is larger than 1 the quasielectron in graphene has the supercritical Coulomb charge. In the opinion this leads to the production of an electron-hole pair via the coupling hole into the initial quasielectron forming a bound state but the emitted quasielectron has again a supercritical charge. Thus the process of creating pairs continues leading to the formation of exciton (chiral) condensate in the stable phase and as a result the quasiparticles acquire a gap. The exciton condensate formation resolves the problem of instability hence a gap generation should take place in a freely standing graphene making it an insulator.

In the paper a theoretical study the both the quantized energies of excitonic states and their wave functions in graphene is presented. An integral two-dimensional Schrödinger equation of the electron-hole pairing for a particles with electron-hole symmetry of reflection is exactly solved. The solutions of Schrödinger equation in momentum space in graphene by projection the two-dimensional space of momentum on the three-dimensional sphere are found exactly. We analytically solve an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with electron-hole symmetry of reflection. In single-layer graphene (SLG) the electron-hole pairing leads to the exciton insulator states. Quantized spectral series and light absorption rates of the excitonic states which distribute in valence cone are found exactly. If the electron and hole are separated, their energy is higher than if they are paired. The particle-hole symmetry of Dirac equation of layered materials allows perfect pairing between electron Fermi sphere and hole Fermi sphere in the valence cone and conduction cone and hence driving the Cooper instability.

In the our paper the particle-hole pair instability for supercritical Coulomb potential is predicted via resonant states with complex number energies. It signifies the existing of the tachyon solutions in Whittaker equations of which can be well known the Heisenberg equations in one-dimensional systems. These one-dimensional systems one can be carbon armchair ribbons in the vicinity of Dirac point in his spectrum within massless Dirac fermions (Majorana fermions).
In the article\textsuperscript{210} we found the three acoustic branches and three optical branches. In the framework our calculations one can conclude that in the K point the acoustic and optical branches have Dirac point similarly to the Dirac cone in graphene and light cone in relativistic physics, where the light velocity is substituted by the Fermi velocity $v_F = 10^6$ m/s and describes by the massless Dirac equation.

In the article\textsuperscript{210} we found the optical ground states of two phonons in graphene in the vicinity of Dirac point. We found the analytical solutions of Schrödinger equations for two coupled phonons in Dirac point of honeycomb lattice. Phonon pair instability for supercritical scaling of honeycomb lattice is predicted via resonant states with complex number energies. It signifies the existing of the tachyon solutions in Schrödinger equations for definition of optical ground states of two phonons of honeycomb lattice.

Optical ground states of two surface plasmon polaritons in graphene in the vicinity of Dirac point phototransitions are found if magnetic field is applied. We found the analytical solutions of Maxwell equations in Majorana form for two coupled surface plasmon polaritons in Dirac point of honeycomb lattice. Surface plasmon polariton pair instability for supercritical scaling of honeycomb lattice is predicted via resonant states with complex number energies. It signifies the existing of the tachyon solutions in Maxwell equations in Majorana form for definition of optical ground states of two surface plasmon polaritons of honeycomb lattice.

\begin{thebibliography}{9}
\bibitem{17} L. E. Lokot, ResearchGate, researchgate.net/profile/Liubov-Lokot/publications (2016).
\bibitem{26} L. E. Lokot, Instability of incommensurate phase of Abrikosov vortex lattice at diffraction metal grating/graphene interface (F1000Physics: Condens. Matter, F1000.com/Workspace, 2016).
\bibitem{28} I. O. Vakarchuk, \textit{Quantum Mechanics} (Ivan Franko Lviv National University, Lviv, 2012), 4th ed.
\bibitem{30} N. Savage, Nature Photonics 1, 83 (2007).
\end{thebibliography}


