Quantum Cryptography

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ACS   https://communities.acs.org/people/LiubovLokot/content

Volume XI

Band energy dispersions from Schrödinger boundary problem for domain wall for data storage of thin PmBaMn$_2$O$_6$ nanofilms

Available online 2 December 2019: https://communities.acs.org/people/LiubovLokot/content

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Abstract In the article we have found the analytical chiral solutions of stationary Schrödinger boundary problem for domain wall for data storage of nanosize PmBaMn$_2$O$_6$ ferroics with incommensurately modulated sinusoidal polarization waves $Q_T$, $Q_P$, $Q_b$. The computer solution of quantized energies or wave vectors of stationary inhomogeneous Schrödinger boundary problem for $Q_T$, $Q_P$, $Q_b$ with sinusoidal depolarization waves for the thin PmBaMn$_2$O$_6$ nanofilm are specified. We have specified the analytical quantized solutions for the band energy dispersion in nanosize ferroics in framework of Landau-Ginsburg-Devonshire (LGD) theory as well as the numerical computer calculation results for the thin PmBaMn$_2$O$_6$ nanofilm have been presented. I think in the article [1] the derived of Phase diagram modeling and domain splitting in thin ferroelectric films with incommensurate phase by A.N. Morozovska et.al. were not allowed and consequently quantized energies or wave vectors were not found by means of the uncertain inference of just these similar symmetrical expressions into (14), (42).

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Spin Hall insulators have connected with respect to dissipationless spin transport via a sample with the spin-orbit interactions (SOI) effects. The extremum rings of the valence band in tensile strained zincblende GaN quantum well as well as the two valley shape of the valence band in GaN nanotube grown along c axis were a collection have attracted our attention both for their fundamental studies and for their device applications. The Quantum Spin Hall effects are shown to be related with intraband transitions of bulk GaN. In the framework of the effective mass theories we have solved the Schrödinger equation if the topological insulator transformation is achieved. The exact solutions of the Schrödinger equations as well as Quantum Spin Hall effect of intraband transitions of bulk GaN are found. For the hexagonal symmetry of GaN the Effective Hamiltonian based on C_{6v} point symmetry group was found. In the article for Quantum Hall effect of intraband phototransitions of bulk GaN the expressions of Berry curvature as well as Hall conductivities have been found when the topological insulator transformation is achieved. Spin Hall insulators have connected with the Topological insulator (TI) as well as Exciton insulators. The dissipationless spin transport via the sample are shown to be related with Spin Hall insulator self-consistent solution of the Schrödinger equations for electrons and holes and the Poisson equations at the presence of spatially varying quantum well potential due to the piezoelectric effect and the local exchange-correlation potential in ZnO quantum well. In ZnO/Zn,MgO quantum well the electron-hole pairing leads to the exciton insulator states. An exciton insulator states with a gap 3.4 eV of ZnO quantum well and at 310 K temperature are predicted. If the electron and hole are separated, their energy is higher on 0.2 meV than if they are paired. The particle-hole pairing leads to the Cooper instability.
2 Introduction

In the article [2, 3, 4, 5] we have found the analytical chiral solutions of stationary Schrödinger boundary problem for domain wall for data storage of nanosize ferroics with incommensurately modulated sinusoidal polarization waves \( P_3 \). The both quantized energies and wave vectors of stationary Schrödinger boundary problem for \( P_3 \) with sinusoidal depolarization waves are specified. We have specified the analytical quantized solutions for the frequency dispersion of soft phonon modes in nanosize ferroics in framework of Landau-Ginsburg-Devonshire (LGD) theory as well as the numerical calculation results for the thin \( \text{SrTiO}_3 \) nanofilm have been presented. The frequency quantized dispersion of soft phonon modes in nanosize ferroics found from stationary Schrödinger boundary problem for domain wall are shown to be related with the Rashba and Dresselhaus quantized energies as well as their wave vectors for electrons in quantized magnetic field. The quantized polarization as well as elastic displacement of stationary Schrödinger boundary problem for domain wall for data storage based on bulk ferroics are found. We have found the quantized solutions of stationarity non-linear high-polynomial Schrödinger or Euler-Lagrange boundary problem for the order parameter as well as elastic displacement in nanosize ferroics. Quantized solutions of one-dimensional Maxwell equations for thin ferroelectric films have been specified which were bonded with stationary solution of cubic and 5-polynomial Schrödinger equation are found. I think in the article [1] the derived of Phase diagram modeling and domain splitting in thin ferroelectric films with incommensurate phase by A.N. Morozovska et.al. were not allowed and consequently were not found by means of the uncertain inference of just these similar symmetrical expressions into (14), (42).

The quantized polarization as well as energy levels solutions of stationary Schrödinger boundary problem for domain wall for data storage based on interface of polar-active ferroelectric nanofilm with semiconductor are found. The self-consistent stationarity quantized solutions of the both like cubic thus 5-polynomial Schrödinger or Euler-Lagrange boundary problem for the polarization vector with one-dimensional Maxwell equations system at interface of thin ferroelectric films and semiconductor in framework of Landau-Ginsburg-Devonshire (LGD) theory theory were presented. We have found the quantized solutions of stationarity non-linear high-polynomial Schrödinger or Euler-Lagrange boundary problem for the polarization vector with one-dimensional Maxwell equations system at interface of thin ferroelectric films and semiconductor. Quantized solutions of one-dimensional Maxwell equations for thin ferroelectric films have been specified which were bonded with stationary solution of cubic and 5-polynomial Schrödinger equation are found. Recently one can see the increasing attentions regarding complex superstructures with incommensurate nature. The optica of the complex superstructures with incommensurate nature has been intensively explored. A particular examples for those complex superstructures were a modulated structures, a structures of charge density waves or spin density waves, an Abrikosov vortex lattice in the crimping films of the superconducting aluminium in the perpendicular magnetic field in which arise the interference between the vortex period caused the magnetic field and the crimping period [2, 3, 4, 5]. To sum up problem of Quantum Field Theory is the instability of incommensurate phase of Abrikosov vortex lattice of graphene and surface plasmon polaritons of diffraction grating/graphene interface in which arise the interference between the vortex period caused the magnetic field and the period of diffraction metal grating.

In the article [6] the group-theoretical methods and first-principles calculations to analyze a set of coupled structural distortions that underlie the polar charge and orbitally ordered antiferromagnetic ground state of A-site ordered \( \text{SmBaMn}_2\text{O}_9 \) have been developed. The authors show that these distortions play a key role in establishing the ground state and stabilizing a network of domain wall vortices.

The polar-active properties of ferroelectric films have been calculated in Landau-Ginsburg-Devonshire theory framework [7, 8, 9, 10, 11, 2, 12, 13, 14, 15, 16, 1] with account of polarization vector gradients and surface charges and dipole layers on the interface in the conditions of stability of spontaneous polarization. Under the electric voltage feeds on the electrode or sound of scanning electron microscope the polarization redistributions have been achieved success. Under the increasing the electric voltage the local reversal of polarizations [17, 15, 16, 1] has been achieved which one...
lied to the creation the intergrown domains in thin films. Under domains recording the velocity of changes of extrinsic electric field $E$ was negligibly small and without loss of accuracy one can suppose $\text{rot}E \approx 0$. In comparison with the tight-binding method the one-component approximation of LGD theory for polarization and displacement allows the calculation only the lowest optic and lowest acoustic soft phonon modes in ferroics. Hence the one-component approximation of LGD theory for polarization and displacement can study quantitatively the soft phonon dispersion in paraelectric SrTiO$_3$. However, the one-component approximation of LGD theory for polarization and displacement cannot calculate the soft phonon dispersion in multiaxial ferroelectric, perovskites BaTiO$_3$ or (Pb,Zr) TiO$_3$ for which the tight-binding method has been applied.

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

Under the spontaneous polarization switching in multiferroic as well as ferroelectric the single domain wall as well as the controlled elements of memory of nanodomain structures with increasing density of nanodomains as well as complicate domain recording of information [17, 15, 16, 1].

It is known [18] vibrations with sine-type modulations can be induced by the impulsive stimulated Raman-scattering process resulting in sine-type oscillations. It explains the coherent oscillations observed in transparent compounds under pumping with a photon energy smaller than an optical gap [18]. In an opaque materials the abrupt modification of pump photons can trigger displaced motions of ions towards new coordinates in the excited state resulting in cosine-type oscillations [18].

The physical properties of wide bandgap group-III quantum well systems are under investigation due to their application to light emitters and semiconductor lasers in the ultraviolet, blue, and green wavelength regions. Ultraviolet light-emitting diodes and lasers have recently obtained considerations due to applications to the compact biological detection systems, analytical devices, and medical diagnostics. A number of light-emitting diodes and laser diodes have been demonstrated [19, 20]. However, these structures are in the developmental stage, and there are many questions with respect to the 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 the data storage. Although such devices basically need a Al$_{x}$Ga$_{1-x}$N-based quantum well with high Al contents, their fundamental optical properties remain under discussion [21, 22, 5, 23, 8, 24, 25, 26, 27, 28, 29, 3, 4, 30]. It has been proved experimentally that the surface emission from [0001]-oriented Al$_{x}$Ga$_{1-x}$N is quite weak because of the predominant optical polarization along the [0001] $c$ direction [31, 32, 33]. The explanation of these effects may be found from the difference of structures of the valence bands in AlN and in GaN. In wurtzite GaN or AlN, the degeneracy of the $p$-like states at the $\Gamma$ 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 one, these splittings lead to the ordering of the valence band in AlN: $\Gamma_7$, $\Gamma_9$, and $\Gamma_7$. Whereas we have $\Gamma_9$, $\Gamma_7$, and $\Gamma_7$ in GaN [34, 35]. Therefore, the topmost of the 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 Al$_{x}$Ga$_{1-x}$N with high (low) Al-content is polarized along (perpendicular to) the $c$ axis. Recently, many studies have been focused on the potential application of nanostructures, such as photonic crystal structures, nanoholes, nanodots, and nanorods [36, 37, 38, 39, 40, 41, 18, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 10, 52, 53, 54, 27, 55]. In the studies of the technology involving the photonic band gap, it seems that, in the case of dielectric rod nanoarrays or nanocolumns [29, 3, 56, 57, 58, 59, 60, 28], a large gap is opened for the TM mode, but not for the TE one [35, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 9]. Thus, with this type of structures for laser applications, the light source in the TM mode is obtained.

In the $c$-plane of InGaN/GaN quantum well systems, the compressive strain is induced in the active layer, and the light is TE-polarized [56, 77, 78, 79]. Furthermore, there is a strong internal electric field caused by the spontaneous and piezoelectric polarization charges at the interfaces of the $c$-plane of the 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 red-shifted [80, 30, 4, 81, 82, 83, 84].

In some studies [85, 58, 7, 57, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95] of interface polarization charges, alloy materials were used to make a better performance. Many works have focused on the nonpolar and semipolar planes [96, 97, 7, 79, 78]. These results have testified that the light emission will be polarized, and the quantum confined Stark effect will be reduced. However, due to a higher cost of the $a$- and $m$-plane substrates, it would be better to use the $c$-plane substrate. In work [89, 90, 98, 99], the $c$-plane of the InGaN/AlGaN quantum well structure was considered instead of that of InGaN/GaN in order to obtain a tensile strain in the quantum well layer. The previous studies and calculations have shown that the $\{Z\}$-like state is generated in nitride materials, if the quantum well layer is under a tensile biaxial strain.

Besides the nitride-based devices, the group-II oxides have been considered for highly efficient laser diodes [98, 99] and high-performance field-effect transistors [100, 101]. The induced piezoelectric field plays a significant role for both band structure and optical gain [102, 103, 104]. However, the orientation of a crystal structure significantly
modifies the band structure through the strain effect [105]. It has been proved experimentally that the 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 [106]. There are the theoretical works studying the effects of crystal orientation on the piezoelectric field in a strained wurtzite quantum well [104]. However, the piezoelectric effect consists not only of a strain-induced polarization; it also takes the response of both electric field and polarization on the strain into consideration. These effects were studied in paper [104].

A deeper understanding of the influence of band structures on optical properties should help one to answer many questions. In addition, the interesting effects of strong electron-hole Coulomb interaction are presented in these materials. Many-body interactions lead to effects, which consist the screening, dephasing, bandgap renormalization, and phase-space filling [107, 108, 109, 110].

A general phenomenon of Coulomb enhancement may be explained as follows. Due to the Coulomb attraction, an electron and a hole have a larger tendency to be located near each other, than that in the case of noninteracting particles. This increase of the interaction duration leads to an increase of the optical transition probability.

In the article the presented phenomena arising from the interplay between the polarity and electronic structure include two dimensional electron gases at the interface of band (LaAlO3/SrTiO3) or band or Mott insulators and polarization controlled electron tunneling across ferroelectric-semiconductor or half-metal interfaces (PtTiO3/(La,Sr)MnO3, BaTiO3/SrRuO3) [10, 11, 16, 15, 111]. The analytical calculations of polar active properties (including local polarization reversal) in the proper and incipient ferroelectric-dielectric thin films within Landau-Ginsburg-Devonshire (LGD) phenomenological theory with consideration of polarization gradient and intrinsic surface energy, interface dipoles, and free charges were presented in the works [10, 11, 16, 15, 111]. Hence the latter works provides a framework to link the mesoscopic LGD semiconductor theory to the first principle calculations that can reveal the details of the electrostatic field structure at the interface.

The optical activity in Rb2ZnBr4, Rb2ZnCl4, K2SeO4, (NH4)2BeF4, (N(CH3)4)2MnCl4 crystals has been measured along three directions in a temperature interval from 400K to 50K [36]. In the incommensurate phase already a nonvanishing element of the gyration tensor has been observed despite the fact that the the average crystal structure has inversion symmetry [36]. In order to explain this phenomenological space dependent dielectric and gyration tensors being invariant with respect to the superspace group of Rb2ZnBr4, Rb2ZnCl4, K2SeO4, (NH4)2BeF4, (N(CH3)4)2MnCl4 have been considered [36, 52, 39, 40, 53, 50, 51, 10].

Recently one has seen a growing interest in systems like modulated crystals with charge or spin density waves which can be considered as crystals with a distortion which is periodic in space or in space time [52, 112, 113, 114, 115, 116, 117, 118, 36, 53]. The Euclidean symmetry of these systems was not a three-dimensional space group but a four-dimensional superspace groups [52, 36, 39, 40, 119, 120, 121, 122, 53, 50, 51, 123, 124].

It is known that the spin-orbit coupling originates from gradients of the Coulomb potentials in the atomic cores [125, 126, 127, 128]. The spin-orbit coupling have been presented by \( \Delta = \frac{\hbar}{2m_{\text{e}} c^2} (\psi_x | \nabla V \times \mathbf{p} | \psi_y) \), where \( V \) is the microscopic crystal potential of graphene. In graphene we would have \( \Delta = 0 \) if the basis functions \( |\psi_x\rangle \) and \( |\psi_y\rangle \) were made up on basis of pure \( \pi \) or \( \sigma \) orbitals. However spin-orbit coupling induces a mixing of the \( \pi \) or \( \sigma \) and \( \sigma \) or \( \pi_\alpha \) orbitals [129] in graphene that contributes to \( \Delta \) in second order of spin-orbit coupling. In the our case [54, 8, 27, 55, 130, 56, 57, 38, 58, 59, 131, 60] the strain mediates a coupling between intrinsic-spin and orbital dynamics and the lowest order contribution \( p_{\Sigma}^{SS}(e_{xx} + e_{yy})s_{\pi}^2s_{\sigma}^2 \) constitutes a renormalization of the intrinsic spin-orbit coupling \( p_{\Sigma}^{SS} \). In the article [37, 42, 132, 43, 143, 134, 97, 96, 45, 46, 47, 48, 49] a creation of giant spin-orbit splitting (\( \sim 100 \text{ meV} \)) of the graphene Dirac cone up to the Fermi energy are shown to be related with Au intercalation at the graphene-Ni interface. Photoelectron spectroscopy [135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149] reveals the hybridization with Au 5d states as the source for this giant splitting. A sharp graphene-Au interface at the equilibrium distance accounts for only \( \sim 10 \text{ meV} \) spin-orbit splitting and enhancement is due to the Au atoms in the hollow position that get closer to graphene and do not break the sublattice symmetry [106, 105, 104, 150, 151, 152, 153, 154, 155, 103, 156, 157, 158, 102, 101, 100, 34, 136, 109, 108, 107].

3 Incommensurately modulated sinusoidal polarization waves \( Q_T, Q_P, Q_b \) in stationary Schrödinger boundary problem for domain wall for data storage of PmBaMn2O6 nanosize ferroics

We have found the following Landau-free energy expansion for specify domain walls for data storage of thin PmBaMn2O6 nanofilms with the P4mm space group of reference data [6, 159]

\[
F_1 = \frac{1}{2} \alpha_1 Q_T^2 + \frac{1}{2} \beta_1 Q_T^4 + \frac{1}{2} \alpha_2 (s_1^2 + s_2^2) + \frac{1}{2} \beta_2 (s_1^2 + s_2^2)^2 + \frac{1}{2} \gamma_1 s_1^2 s_2^2 + \frac{1}{2} \alpha_3 Q_b^2 + \frac{1}{2} \alpha_P Q_P^2 + F_{tss} + F_{bsb} + F_{tBP},
\]

where \( F_{tss} = \delta_{tss} Q_T s_1 s_2, F_{bsb} = \delta_{bsb} Q_b (s_1^2 - s_2^2), \) as well as \( F_{tBP} = \delta_{tBP} Q_T Q_b Q_P \).
Figure 1. (Color online) Dispersion of quantized energy spectrum $Q_T$ of stationary Schrödinger boundary problem for domain wall for data storage of nanosize ferroics PmBaMn$_2$O$_6$ with ferroelectric nanofilm width $h = 2$ nm.

Figure 2. (Color online) Dispersion of quantized energy spectrum $Q_P$ of stationary Schrödinger boundary problem for domain wall for data storage of nanosize ferroics PmBaMn$_2$O$_6$ with ferroelectric nanofilm width $h = 2$ nm.
Figure 3. (Color online) Dispersion of quantized energy spectrum $Q_T$ of stationary Schrödinger boundary problem for domain wall for data storage of nanosize ferroics PmBaMn$_2$O$_6$ with ferroelectric nanofilm width $h = 20$ nm.

Figure 4. (Color online) Dispersion of quantized energy spectrum $Q_P$ of stationary Schrödinger boundary problem for domain wall for data storage of nanosize ferroics PmBaMn$_2$O$_6$ with ferroelectric nanofilm width $h = 20$ nm.
The Euler-Lagrange dynamic equations for the order parameter component \( Q_T (k_x, z) \) further denoted as \( f_k (k_x, z) \equiv \phi (k_x, z, k_y) \) we have specified from the Lagrange function of ferroic film by varying of variables of the Functional Eq. (1)

\[
\begin{align*}
\alpha_s Q_T + \beta_t Q_T^2 + \delta_{1s} s_1 s_2 + \delta_{1b} P Q_b Q_p &= 0, \\
\alpha_s Q_b + \delta_{1b}(s_1^2 - s_2^2) + \delta_{1p} P Q_T &= 0, \\
\alpha_p Q_p + \delta_{1b} P Q_T Q_b &= 0,
\end{align*}
\]

(2)

where \( s_1^2 + s_2^2 = Q_z^2, s_1 = 0.88 Q_z, s_2 = 0.47 Q_z, Q_z^2 + Q_s^2 + Q_t^2 + Q_r^2 = 1. \)

From equations system Eqs. (2) one can find

\[
\alpha_s Q_b + \delta_{1b} P Q_T Q_b = 0,
\]

(3)

the order parameter \( Q_b \)

\[
Q_b = -\frac{\alpha_s Q_T}{\delta_{1b} P Q_T},
\]

(4)

and substituting \( Q_b \) in Eqs. (2) we have derived

\[
-\frac{\alpha_s a_s Q_p}{\delta_{1b} P Q_T} + \delta_{1b} P Q_T Q_p + \delta_{1b}(s_1^2 - s_2^2) = 0,
\]

(5)

as well as

\[
-\alpha_s Q_p + \delta_{1b} P Q_T Q_p + \delta_{1b}(s_1^2 - s_2^2) \delta_{1b} P Q_T = 0,
\]

(6)

and after elementary transformations one can find

\[
Q_p(-\alpha_s a_h + \delta_{1b} P Q_T^2) = \delta_{1b}(s_2^2 - s_1^2) \delta_{1b} P Q_T.
\]

Hence we have found

\[
Q_p = \frac{\delta_{1b}(s_2^2 - s_1^2)}{(-\alpha_s a_h + \delta_{1b} P Q_T^2)},
\]

(8)

as well as

\[
Q_b = -\frac{\alpha_s a_h}{(-\alpha_s a_h + \delta_{1b} P Q_T^2)}.
\]

(9)

Substituting Eqs. (8), (9) into Eqs. (2) we have specified the equation for \( Q_T \) order parameter as follows

\[
\begin{align*}
\alpha_s Q_T + \beta_t Q_T^2 + \delta_{1s} s_1 s_2 - \frac{\alpha_s a_h}{(-\alpha_s a_h + \delta_{1b} P Q_T^2)} = 0,
\end{align*}
\]

(10)

after elementary transformation we have obtained

\[
(\alpha_s Q_T + \beta_t Q_T^2 + \delta_{1s} s_1 s_2)(-\alpha_s a_h + \delta_{1b} P Q_T^2)^2 - \alpha_s a_h \delta_{1b}(s_1^2 - s_2^2)^2 \delta_{1b} P Q_T = 0,
\]

(11)

as well as

\[
(\alpha_s Q_T + \beta_t Q_T^2 + \delta_{1s} s_1 s_2)(a_h^2 a_h^2 - 2 \alpha_s a_h \delta_{1b} P Q_T^2 + \delta_{1b} P Q_T^2) - \alpha_s a_h \delta_{1b}(s_1^2 - s_2^2)^2 \delta_{1b} P Q_T = 0,
\]

(12)

and hence

\[
\begin{align*}
\alpha_s a_h^2 Q_T - 2 \alpha_s a_h \delta_{1b} P Q_T^3 + \alpha_s a_h^4 Q_T^2 + \alpha_s a_h^2 \beta_t Q_T^2 - 2 \alpha_s a_h \beta_t \delta_{1b} P Q_T^2 + \beta_t \delta_{1b} P Q_T^2 + \\
+ \delta_{1s} s_1 s_2 a_h^2 \alpha_p - \delta_{1b} \delta_{1b} P Q_T + \delta_{1s} s_1 s_2 a_h^2 \alpha_p - \alpha_p \delta_{1b}(s_1^2 - s_2^2)^2 \delta_{1b} P Q_T = 0.
\end{align*}
\]

(13)

Let us known a ferroic film of thickness \( h \) confined in the z direction in the region \( z \in [-h/2, h/2], \) hence \( k_z \rightarrow \frac{-i}{\sqrt{h}} \).

The film surfaces are covered by two ideally conducting soft electrodes, which do not affect its mechanical state and we have specified the nanofilm by the wave vectors in the space with orthonormal basis \([1, \zeta_r]\) like as

\[
\Psi_{1, \zeta_r} = |v_{\zeta_r} k_z\rangle = \sum_{i=1}^{m} \psi^{(1)}_{i, \zeta_r} |v_{\zeta_r} k_z\rangle = |1, \zeta_r\rangle,
\]

(14)

where \( \zeta_r \) is a chirality, \( \psi(Z) = \sqrt{\frac{1}{N}} \sin (\pi m (\frac{z}{h} + \frac{1}{2})) = \sqrt{\frac{1}{N}} \sin (\pi m Z), Z = (\frac{z}{h} + \frac{1}{2}). \)

We have specified the depolarization field \( E_{\phi}^d [f_k (k, z)] \) by Eq. (15) and which has been involved into Schrödinger boundary problem Eqs. (28), (29) determines the chirality form of solution of Eqs. (28), (29).
Figure 5. (Color online) Dispersion of quantized energy spectrum $Q_T$ of stationary Schrödinger boundary problem for domain wall for data storage of nanosize ferroics PmBaMn$_2$O$_6$ with ferroelectric nanofilm width $h = 50$ nm.

Figure 6. (Color online) Dispersion of quantized energy spectrum $Q_T$ of stationary Schrödinger boundary problem for domain wall for data storage of nanosize ferroics PmBaMn$_2$O$_6$ with ferroelectric nanofilm width $h = 50$ nm.
\[
\hat{E}_\alpha^2[Q_T(k,\alpha)] = \left\{ \frac{\hat{Q}_r(k_s) + \int_k^z dq \frac{q-r}{|q-r|} \hat{Q}_r(k,\alpha) \sin[K(q-r)] |(K(k) - \sin(k\alpha)) [\cos(kh)]} {\int_k^z dq \frac{q-r}{|q-r|} \hat{Q}_r(k,\alpha) \sin[K(q-r)] |(K(k) - \sin(k\alpha)) [\cos(kh)]} \right\}.
\]

In the simplest one-component one-dimensional case considered hereafter, the bulk part of the free energy \( F \) which depends on one-component order parameter \( Q_T \) coupled with the order parameters \( Q_b \) when \( Q_p \) which depend only on the coordinate \( x \) and their gradients has the following form

\[
F \approx \int_0^h dz \int_{-\infty}^{\infty} dxdy \left\{ \frac{1}{2} \alpha_t Q_T^2 + \frac{1}{2} \beta_t Q_T^2 + \frac{1}{2} \alpha_b (s_1^2 + s_2^2) + \frac{1}{2} \beta_b (s_1^2 + s_2^2) + \frac{1}{2} \alpha_i Q_b^2 + \frac{1}{2} \beta_i Q_b^2 + \frac{1}{2} \alpha_p Q_p^2 + F_{ba} + F_{hp} + F_{tb} - \frac{1}{2} Q_T^2 + E_0 \right\}
\]

(16)

where

\[
Q_p = \frac{\delta_{\alpha b}(s_1^2 - s_2^2) s_{1a} Q_T}{\alpha_{12} \alpha_{21} Q_T},
\]

(17)

\[
Q_b = -\frac{\delta_{\alpha b}(s_1^2 - s_2^2) s_{1a} Q_T}{\alpha_{12} \alpha_{21} Q_T},
\]

(18)

as well as \( \alpha_t = \alpha(T) - \frac{(Q_1 + \Delta Q_1)^2}{s_{11} + s_{12}} - 2 \frac{(Q_1 + \Delta Q_1)^2}{s_{11} - 2s_{12}Q_1 + \Delta Q_1} \frac{s_{12}}{s_{11}} \), \( \beta_t = \beta + 2 \frac{(Q_1 + \Delta Q_1)^2}{s_{11} - 2s_{12}Q_1 + \Delta Q_1} \), \( s_{ij} \) is an elastic coefficients. Hence we have specified the stationary Schrödinger boundary problem in space confined medium or planar waveguide as follows

\[
\Gamma \frac{\partial Q_T}{\partial r} + \alpha Q_T + \alpha \beta Q_T^2 + \beta \gamma Q_T^4 + \gamma \beta Q_T^2 + \gamma \gamma Q_T^2 + \gamma \gamma Q_T^2 - g_3 \frac{\partial Q_T}{\partial r}^2 - (g_1 + \delta T_1 s_1) \frac{\partial Q_T}{\partial r}^2 + \frac{\partial^2 Q_T}{\partial x^2} + \frac{\partial^2 Q_T}{\partial y^4}) - \nu_1 Q_T \left[ \frac{\partial Q_T}{\partial x}^2 + \frac{\partial Q_T}{\partial y}^2 \right] + \delta_{11} s_1 s_2 \alpha_{1}^2 \beta_{1}^2 = E_0(x, y, z) + E_0 \exp(\omega t),
\]

(19)

where

\[
\alpha^* = \alpha \alpha_{12} \alpha_{21} - \alpha \beta_{12} \beta_{21} \left( s_1^2 - s_2^2 \right)^2 \beta_{12}^2,
\]

(20)

\[
\alpha' = -2 \alpha \alpha_{12} \beta_{12} \beta_{21} s_1 s_2 \beta_{12}^2,
\]

(21)

\[
\beta^* = -2 \alpha \alpha_{12} \beta_{12} \beta_{21} \alpha_{12}^2 \beta_{12}^2,
\]

(22)

\[
\beta' = \delta_{11} s_1 s_2 \beta_{12}^4,
\]

(23)
\[
\gamma' = \alpha \delta_{t \beta p}^4 - 2 \alpha \beta \alpha_3 \beta_2 \delta_{t \beta p}^2, \tag{24}
\]
\[
\gamma' = \beta \delta_{t \beta p}^4, \tag{25}
\]
and with boundary conditions
\[
(\alpha' Q_T - g_3 \frac{\partial Q_T}{\partial x_3} - w_1 \frac{\partial Q_T}{\partial x_2} - v_1 Q_T \frac{\partial Q_T}{\partial x_3}(Q_T + \frac{\partial Q_T}{\partial x_3}))|_{x_3 = 0} = 0,
\]
\[
(\alpha' Q_T + g_3 \frac{\partial Q_T}{\partial x_3} + w_1 \frac{\partial Q_T}{\partial x_2} + v_1 Q_T \frac{\partial Q_T}{\partial x_3}(Q_T + \frac{\partial Q_T}{\partial x_3}))|_{x_3 = h} = 0. \tag{26}
\]

The solutions of the stationary Schrödinger boundary problem in space confined medium or planar waveguide in the form of expansion into a series
\[
p(k, z, t) = \sum_{n, j} [\psi^{(j)}_k[i, v] \psi_n(Z)] j, \zeta \exp(-\lambda_n(k)Z^2) + E_n(k, \omega) \frac{f(k, x) \exp(\alpha x t)}{\lambda_n(k) + \alpha x t}. \tag{27}
\]
Euler-Lagrange equations which linearized with respect to the polarization and displacement fluctuations acquire the following form in two-dimensional \( k_i = \sqrt{k_\parallel^2 + k_\perp^2} \) space
\[
(\alpha' f_n - g_3 \frac{\partial f_n}{\partial x_3} - w_1 \frac{\partial f_n}{\partial x_2} - v_1 f_n \frac{\partial f_n}{\partial x_3}(f_n + \frac{\partial f_n}{\partial x_3}))|_{z = 0} = 0,
\]
\[
(\alpha' f_n + g_3 \frac{\partial f_n}{\partial x_3} + w_1 \frac{\partial f_n}{\partial x_2} + v_1 f_n \frac{\partial f_n}{\partial x_3}(f_n + \frac{\partial f_n}{\partial x_3}))|_{z = h} = 0. \tag{28}
\]

The Euler-Lagrange dynamic equations for the order parameter component \( Q_T(k_i, z) \) further denoted as \( f_p(k_i, z) \equiv \Phi^{(j)C}_v(z, k_i) \) we have specified from the Lagrange function of ferroic film by varying of variables of the Functional. The boundary conditions for \( f_p(k_i, z) \) have the form
\[
(\alpha' f_n - g_3 \frac{\partial f_n}{\partial x_3} - w_1 \frac{\partial f_n}{\partial x_2} - v_1 f_n \frac{\partial f_n}{\partial x_3}(f_n + \frac{\partial f_n}{\partial x_3}))|_{z = 0} = 0,
\]
\[
(\alpha' f_n + g_3 \frac{\partial f_n}{\partial x_3} + w_1 \frac{\partial f_n}{\partial x_2} + v_1 f_n \frac{\partial f_n}{\partial x_3}(f_n + \frac{\partial f_n}{\partial x_3}))|_{z = h} = 0 \tag{29}
\]
where \( f_p(k_i, z) \equiv \Phi^{(j)C}_v(z, k_i) = \sum_{n=1}^m \Psi^{(j)}_k[n, v] \psi_n(Z), j = 1, 2 \), where also \( \tilde{n} \) from \([1]\) i.e. \( \psi^{(j)}_k[n, v] \psi_n(Z) \) = \( (\tilde{f}) \).

The solutions of Schrödinger equations can be found in the form Eq. (14) i.e. \( \Phi^{(j)C}_v(z, k_i) = \sum_{n=1}^m \Psi^{(j)}_k[n, v] \psi_n(Z), j = 1, 2 \) by premultiply the equations system of Eq. (28) on \( \psi_n(Z) \) functions and by integrating the later equations system on quantum box boundaries.

Let us known the following integral relations for the found solutions algebra equation systems
\[
\int_0^1 h \psi(n, Z) \psi(n, Z) dZ = 1, \tag{30}
\]
\[
\int_0^1 h \psi(n, Z) \psi(k, Z) dZ = 0, \tag{31}
\]
if \( n \neq k \),
\[
\int_0^1 \psi(n, Z) \frac{\partial \psi(n, Z)}{\partial Z} dZ = -\frac{k((-1)^n(-k+n)+(-1)^n(n-k)-2n)}{(n+k)(n-k)h}, \tag{32}
\]
if \( n = k \),
\[
\int_0^1 \psi(n, Z) \frac{\partial \psi(n, Z)}{\partial Z} dZ = 0, \tag{33}
\]
\[
\int_0^1 \psi(n, Z) \frac{\partial \psi(n, Z)}{\partial Z} dZ = -\frac{\pi^2 n^2}{h}. \tag{34}
\]
Since
\[
\int_0^1 \psi(n, Z) \frac{\partial \psi(n, Z)}{\partial Z} dZ = -\frac{\pi^2 n^2}{h}, \tag{35}
\]
then we have replaced \( k^2_m \rightarrow -\frac{\pi^2 n^2}{h} \) in Eq. (28), keeping in the mind that the solutions of Schrödinger equations can be found in the form Eq. (14) i.e. \( \Phi^{(j)C}_v(z, k_i) = \sum_{n=1}^m \Psi^{(j)}_k[n, v] \psi_n(Z), j = 1, 2 \) by premultiply the equations system of Eq. (28) and hence the depolarization fields Eq. (15) on \( \psi_n(Z) \) functions and by integrating the later equations system on quantum box boundaries one can find
\[
\int_0^1 \sin(\pi n Z) \sin(kh(Z - \frac{1}{2})) \sin(\pi n Z) dZ = 0, \tag{36}
\]
\[
\int_0^1 \sin(\pi n Z) \sin(kh(Z - \frac{1}{2})) \sin(\pi m Z) dZ = 0. \tag{37}
\]
\[ \psi_i'(Z) = \frac{1}{\sqrt{2 \pi}} \frac{e^{i \pi nZ} \sin(Kh(1-Z)) \sin(\pi nZ)}{K/(\pi - \pi^2 n^2)} \]

with the following approximation of matching of quasi-classical functions

\[ \frac{\pi n^2 \cos(\pi nZ)}{\pi^2(2m^2-k^2h^2)} \approx \frac{\pi m^2 \cos(\pi mZ)}{\pi^2(2m^2-k^2h^2)} \frac{\sin(\pi n)\sqrt{\eta} + i \pi n \cos(\pi n)}{\sin(\pi m)\sqrt{\eta} + i \pi m \cos(\pi m)}, \]

we have found the quasi-exactly stationary Schrödinger boundary problem for wave vectors \( \psi_k^{(j)} [n, \nu] \) of quantized band energy dispersions

\[ \Psi_k^{(j)} [n, \nu] = ([(\alpha^* + g_1 k_1^2 + w_1 k_4^4 - g_3 \frac{\pi^2 n^2}{h^2} + \frac{\pi^2 n(1 - \cos(Kh)) \tan(Kh)}{e_{\nu, s} n(\pi(2m^2-k^2h^2))} \delta_{nm} + K \tan(kh) \frac{2 \pi m n K \cos(Kh) + (-1)^{n(s+1)}}{K/(\pi - \pi^2 n^2)}])^{-1} \delta_{1s_1 s_2} \delta_{1s_1 s_2} \alpha_f^2, \]

where \( h = 1, \nu \equiv \tilde{n} \) does not coincide with \( n, \alpha^* = \alpha^* + 2\alpha' Q_T + 3\beta' (Q_T)^2 + 4\beta' (Q_T)^3 + 5\gamma' (Q_T)^4 + 7\gamma' (Q_T)^5, \)

\[ g_1 = g_1 + v_1 (Q_T)^2, \]

\[ Q_T = \text{the average order parameter (for a bulk single domain sample the averaged order parameter } \langle Q_T \rangle^2 = (\sqrt{B^2 - 4a^2 r^2 - \beta^2)/2} \gamma^2) \text{.} \]

[1] We have specified the depolarization field \( E_{ij} [f_0 (k_i, z)] \) by Eq. (15) and which has been involved into Schrödinger boundary problem Eqs. (28), (29) determines the chirality form of solution of Eqs. (28), (29). Hence in addition identically true the following dispersion expressions for star of wave vector \( s_1 = 0.88 + Q_s, s_2 = 0.47 + Q_s, \) where \( Q_s \equiv \kappa_s, \) the dispersion region \( M_s^+ \rightarrow M_s^+ \) we have specified as \( s_1 = 0.88 + 3/3 + Q_s \) as well as \( s_2 = 0.47 + 3/3 + Q_s, \) the dispersion region \( M_s^+ \rightarrow \Sigma_s^2 \) we have specified as \( s_1 = 0.88 + 2/3 + Q_s, \) as well as \( s_2 = 0.47 + 2/3 + Q_s, \) and the dispersion region \( \Gamma_s^2 \) has been found as \( s_1 = 0.88 + Q_s, s_2 = 0.47 + Q_s, \) where \( Q_s \equiv \kappa_s. \)

I think in the article [1] the derived of Phase diagram modeling and domain splitting in thin ferroelectric films with incommensurate phase by A.N. Morozovska et.al. were not allowed and consequently the quantized band energies were not found by means of the uncertain inference of just these similar symmetrical expressions into (14), (42).

### Table 2. Material parameters for \( S_2P_2Se_6 \) [10, 11, 15, 16, 1, 111]

<table>
<thead>
<tr>
<th>Description</th>
<th>Symbol and dimension</th>
<th>Incipient ferroelectric ( S_2P_2Se_6 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Curie-Weiss constant</td>
<td>( \alpha_T \times 10^6 \text{Jm} / \text{C}^2 \text{K} )</td>
<td>1.6</td>
</tr>
<tr>
<td>Curie temperature</td>
<td>( T_C \text{ (K)} )</td>
<td>193</td>
</tr>
<tr>
<td>LGD-coefficient at ( 4^4 )</td>
<td>( \beta \times 10^3 \text{J}^4 \text{C}^{-6} \text{m}^5 )</td>
<td>-4.8</td>
</tr>
<tr>
<td>LGD-coefficient at ( 6^6 )</td>
<td>( \gamma \times 10^3 \text{J}^4 \text{C}^{-6} \text{m}^5 )</td>
<td>8.5</td>
</tr>
<tr>
<td>Gradient coefficient at ((\nabla \eta)^2)</td>
<td>( g_1 \times 10^{-10} \text{C}^{-2} \text{m}^3 \text{J} )</td>
<td>-5.7</td>
</tr>
<tr>
<td>Kinetic coefficient</td>
<td>( w_1 \times 10^{-27} \text{Jm}^5 / \text{C}^2 )</td>
<td>1.8</td>
</tr>
<tr>
<td>Kinetic coefficient</td>
<td>( v_1 \times 1.6 \times 10^{-8} \text{Jm}^5 / \text{C}^2 )</td>
<td>1.2</td>
</tr>
<tr>
<td>Kinetic coefficient</td>
<td>( g_3 \times 10^{-10} \text{Jm}^3 / \text{C}^2 )</td>
<td>5</td>
</tr>
<tr>
<td>Material permittivity</td>
<td>( \varepsilon_{11} = \varepsilon_{33} )</td>
<td>10</td>
</tr>
<tr>
<td>Material permittivity</td>
<td>( \varepsilon_0 )</td>
<td>9.38</td>
</tr>
</tbody>
</table>

In Figs. 1-7 we have presented the computation solutions of quantized energies of the Eq. (42) stationary Schrödinger boundary problem for different thickness \( h \) of \( \text{PmBaMn}_2\text{O}_6 \) ferroelectric nanofilms.

### References


Material parameters in Landau free-energy expansion for PmBaMn$_2$O$_6$ [6].

<table>
<thead>
<tr>
<th>Symbol and dimension</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_4$ (eV/Å$^2$)</td>
<td>-0.29</td>
</tr>
<tr>
<td>$\alpha_5$ (eV/Å$^2$)</td>
<td>2.77</td>
</tr>
<tr>
<td>$\alpha_6$ (eV/Å$^2$)</td>
<td>1.28</td>
</tr>
<tr>
<td>$\beta_1$ (eV/Å$^4$)</td>
<td>0.53</td>
</tr>
<tr>
<td>$\delta_{s\alpha}$ (eV/Å$^3$)</td>
<td>-0.45</td>
</tr>
<tr>
<td>$\delta_{b\alpha}$ (eV/Å$^3$)</td>
<td>-1.46</td>
</tr>
<tr>
<td>$\delta_{t\beta}$ (eV/Å$^3$)</td>
<td>-0.26</td>
</tr>
</tbody>
</table>


