Mathematical modelling and self-consistent calculation of the charge density of two-dimensional electron's system.

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Abstract.

The mathematical model of the 2D-system of electrons in the subsurface space of the homogeneous narrow-gap semiconductor was developed for accumulation layers. The calculation of the 2D-systems parameters was carried out by numerical self-consistent integration of the Schrödinger and Poisson equations by using the Fermi and quasi-classical (WKB) descriptions of the eigenfunctions of the continuous spectrum - the states of electrons "in continuum".

It is shown that the quasi-classical approximation is preferable in comparison with the Fermi one for the description of the continuum for 2D-systems. The parameters of the two-dimensional gas were computed in wide range of temperatures (200—300 K) and potentials (0—0.2 V). There exists possibility of experimental observation of quantum subbands in accumulation layers in the subsurface space of the narrow-gap semiconductor at room temperature.

1 Introduction.

The implementation of quantum gates remains one of the most actual theoretical and experimental problem of nanoelectronics. The design of quantum gates which would posess necessary properties (step-wise shape of voltage-current characteristics , temperature stability ...) requires profound mathematical analysis of the corresponding scattering problem on quantum wire. On the other hand this analysis must be supported by mathematical modelling and experiment.

In [1,2,8] a new class of quantum gates was suggested. Theoretically this gate must reveal stable performance at nitrogen temperatures. Using the dimensional quantization in the subsurface layer of certain semiconducting materials one can rise the range of stable performance to high nitrogen or even room temperatures. The implementation of this gates requires a thorough investigation of dimensional quantization of electrons in subsurface space of a sample of semiconductor shaped in form of a rectangular edge. Our paper is aimed to the modelling of the properties of the two-dimensional electron system in the subsurface space of the sample. Generally the investigation of distribution of electrons or holes in the subsurface layer of a semiconductor in presence of an exterior electrostatic field is a sophisticated few-body spectral problem, which can not be reduced to the straightforward spectral analysis of one-body Schrödinger Operator. Nevertheless a procedure can be developed, which permitts to describe the energy-level's distribution as a result of a sequence of *selfconsistent calculations*.

The exterior electric field can be considered on the first step as a perturbation of the lattice potential of the solid. Thus it affects the Bloch-type eigen-functions of the corresponding *one-body* Schrödinger operator. On the other hand the positive electric potential applied at the surface of the semiconductor causes an increment of the density of electrons in the sub-surface space. In turn this creates efficiently an additional electrostatic potential which can be calculated as a solution of the Poisson equation with the proper density.This density can be derived from the solution of the initial *one-body* spectral problem on the first step. Inserting this additional potential into the Schrödinger equation, we get a *corrected* spectral picture on the second step, which enables us to calculate the corresponding charge density and the corrected electrostatic potential on the second step, and so on.

One usually assumes that only the states of discrete spectrum contribute to the effective charge density. This point of view is obviously noncomplete for quantum gates, in presence of the current, since the charge of conductivity electrons — the electrons in the "continuum" — should be taken into account as well. The problem of the calculation of the contribution of the states of the continuous spectrum into the effective density requires the calculation of the eigenfunctions of the continuous spectrum on each step of the procedure.

In this paper we compare two simplified version of incorporating the eigenfunctions of the continuous spectrum:

a) replacing these eigenfunctions just by exponentials. This permits to reduce the problem immediately to the use of the classical Fermi distribution, or

b) using a quasiclassical asymptotics for eigenfunstions of the continuous spectrum.

The second approach permitts to take into account the important fact of *vanishing of* *wave functions* of conductivity electrons in the surrounding vacuum and at the surface of the semiconductor. Comparing results we get under these assumption we conclude, that the second approach is essentially more informative, supplying the important data on dependence of the additional density and the potential of the spatial coordinates.

The vanishing of the wave functions at the surface of semiconductor is related to the fact, that the lattice potential has a jump at the surface. It was noticed in [2], that this jump is determined by the electron's output-work function. In semiconductors the output-work *exceeds significantly a characteristic energy of electron at the bottom of the conductivity band.* Therefore the wave function of the conductivity electron can be assumed equal to zero outside the solid, thus it should have *a knot* at the surface. In particular it means, that the electron density decreases in the nearest subsurface layer, the width of it approximately equal to the typical de-Broglie wavelength. In turn it results in broadening of the corresponding potential well and growing the density of bound states which reveals in course of more precise description of the corresponding dimension quantization picture (see below).

In actual work we formulate the principles of the mathematical modelling of the system of electrons and charge density in the subsurface space and present the algorithm and the results of calculation of electron properties of the 2D-system in the subsurface space of the antimonide indium. The spectra of bound states and charge densities calculated with use of classical Fermi distribution and quasi-classical (WKB) method are compared.

2 The principles of mathematical modeling of charge density in the subsurface space of the semiconductor.

At present the most efficient approach to the description of multielectron system in a subsurface domain of a semiconductor is the Hartree approximation [1]. It means, that the multielectron system is considered as a one-electrone system in the proper *mean electrostatic potential*, formed by the initial potential U and the additional potential V caused by the charge density , defined by the spectral picture of the same one-electron system. In this approximation the one-particle Schrödinger equation can be written in the form:

$$\left(-\frac{\hbar^2}{2m_e^*}\vec{\nabla}^2 + qU(\vec{r}) + qV(\vec{r})\right)\Psi(\vec{r}) = E\Psi(\vec{r}) \tag{1}$$

with the boundary conditions on the surface $\Psi = 0$. Here m_e^* is the effective mass of the electron in the semiconductor, $\vec{r} = (x, y, z)$. $\hbar$ is the Plank constant (we use the International System of Units (SI) hereafter). In parabolic approximation the law of dispersion reads:

$$E(\vec{k}) = \frac{\vec{k}_r^2\hbar^2}{2m^*}. \tag{2}$$

where $\vec{k}_r$ is the momentum vector and $m^* = (m_x, m_y, m_z)$ is effective mass of free charge carriers.

Let us consider a semi-infinite 2D crystal with an ideal (up to the surface $x = 0$) periodic crystal lattice in $x > 0$. The exterior electrostatic field is applied orthogonaly to the surface, forming a potential well in the subsurface space for electrons with the potential $qU + qV(x)$ defined by the sum of the exterior potential and the potential of the corresponding mean field caused by the induced density. Conversely , for holes the resulting potential has a form of a potential barrier which can be formally incorporated in V . The bound states of electrons with energies ε_n $(n = 1, 2, \ldots)$ appear in this well. The movement of electrons in this states along x-axis is prohibited and the motion of electrons along the YZ-plane is free, so that the one-electron's wave function Ψ can be represented as:

$$\Psi(\vec{r}) = e^{i(k_y y + k_z z)} \varphi_n(x), \tag{3}$$

The "envelope" wave function φ_n is found from the one-dimensional Schrödinger equation:

$$\left(-\frac{\hbar^2}{2m_e^*} \frac{\partial^2}{\partial x^2} + qU(x) + qV(x) \right) \varphi_n(x) = \varepsilon_n \varphi_n(x) \tag{4}$$

with the boundary conditions $\varphi_n(0) = \varphi_n(\infty) = 0$. The total energy of the electron can be represented in the form:

$$E = \varepsilon_n + \frac{k_y^2 \hbar^2}{2m_y^*} + \frac{k_z^2 \hbar^2}{2m_z^*}. \tag{5}$$

In what follows we assume for the sake of simplicity that all effective masses are the same: $m_x^* = m_y^* = m_z^* \equiv m_e^*$. If the eigenfunctions of the Schr̈dinger operator (4) are found, then the corresponding charges densities can be calculated, see below (12, 18). Then the additional potential energy $qV(x)$ in the equation (4) should satisfy the Poisson equation:

$$\frac{\partial^2 V(x)}{\partial x^2} = -\frac{\rho_e(x) + \rho_h(x)}{\varepsilon_0 \varepsilon_{sc}}, \tag{6}$$

where $\rho_e(x)$ and $\rho_h(x)$ are the charge densities of electrons and holes, respectively, which depend only on the x, and $\varepsilon_0,\ \varepsilon_{sc}$ are the permittivity vacuum and semiconductor.

The boundary conditions for the potential in (6) read as $V(0) = V_s$, $V(\infty) = 0$.

The problem of the construction of the solution of the pair of equations (4,6) is a nonlinear one. The important part of it is the construction of the eigenfunctions of the Schr̈dinger operator with the potential $U + V$ and the subsequent calculation of the electron's densities.

One can suggest two approaches to this problem. The first (classical one) is based on the standard Fermi description of the distribution of charge carriers and exponential form of the corresponding eigenfunctions. This approach is not compatible with the boundary condition at the plane $x = 0$. Another possible approach involves the *quasiclassical* description of wave functions of the continuous spectrum , which permits to incorporate the boundary condition as well as the shape of the total potential on the previous step in explicite form. This approximation for the wave functions is valid if both exterior field U and induced field V are varying slowly on intervals comparable with the De-Broghlie wave length of the charge carriers, that is when the quantum objects can be considered as *particles*, not waves. This is certainly true for hole, which has in our case rather large effective mass. For this reason we use for holes just the classical Fermi description of induced density, when the eigenfunctions are represented by exponentials. For electrons we use slightly more precise quasiclassical description.

Thus, the total density of electron charge on the surface of semiconductor is calculated by two method:

— in the first one the electron density of charge in the continuum ($\rho_c^{fermi}(x)$), which is constant in the whole volume of the crystal, combines with the electron density in bound states ($\rho_q(x)$)

$$\rho_e^{fermi}(x) = \rho_c^{fermi}(x) + \rho_q(x), \tag{7}$$

— in the second one the total electron density consists of the electron charge density in the continuum ($\rho_c^{wkb}(x)$) calculated by the quasi-classical approximation (WKB) (see below (18)) and the contribution from the discrete spectrum

$$\rho_e^{wkb}(x) = \rho_c^{wkb}(x) + \rho_q(x). \tag{8}$$

The classical representation for the charge density of electrons and holes (in both methods) in the continuum reads [1]:

$$\rho_c^{fermi}(x) = qN_c F_{1/2}\left(\frac{E_f}{kT}\right), \tag{9}$$

$$\rho_h(x) = qN_v F_{1/2}\left(\frac{-E_f - E_g + qU + qV(x)}{kT}\right), \tag{10}$$

where

$$N_c = 2\left(\frac{2m_e^*\pi kT}{h^2}\right)^{3/2}, \quad N_v = 2\left(\frac{2m_h^*\pi kT}{h^2}\right)^{3/2}, \quad F_{1/2}(x) = \frac{2}{\sqrt{\pi}}\int\limits_0^\infty \frac{\varepsilon^{1/2}\,d\varepsilon}{1+e^{\varepsilon - x}},$$

and m_h^* is the effective mass of the hole, N_c, N_v are the effective densities of the states of the conductivity and valence bands, respectively, and $F_{1/2}(x)$ is the integral Fermi. The position of the Fermi level (E_f) can be determined from the electroneutrality equation for the total charge in the space of the semiconductor:

$$N_c F_{1/2}\left(\frac{E_f}{kT}\right) - N_v F_{1/2}\left(\frac{-E_g - E_f}{kT}\right) = 0. \tag{11}$$

The charge density of electrons in the discrete spectrum of bound states is calculated via the eigenfunctions in the following form:

$$\rho_q(x) = q\sum_n \Gamma(\varepsilon_n)|\varphi_n(x)|^2, \tag{12}$$

$$\Gamma(\varepsilon) = 2\int f(E)\frac{dk_y dk_z}{(2\pi)^2} = \frac{m_e^* kT}{\pi\hbar^2}\ln\left(1+\exp\left(\frac{E_f - \varepsilon}{kT}\right)\right). \tag{13}$$

The function $\Gamma(\varepsilon)$ describes the population of levels with energy ε (the factor of 2 takes into account the spin degeneracy of the states) and is related to the Fermi electron distribution function $f(E)$:

$$f(E) = \frac{1}{1+\exp\left(\frac{E-E_f}{kT}\right)}. \tag{14}$$

The contribution of the continuum to the induced charge density is generally represented as:

$$\rho^{wkb}(x) = q \int\limits_{-\infty}^{\infty} \frac{dk_x}{2\pi} \Gamma(\varepsilon)\ |\varphi_\varepsilon(x)|^2, \tag{15}$$

or after substituting the dispersion law as in (2) can be rewritten in form:

$$\rho^{wkb}(x) = q\frac{\sqrt{2m_e^*}}{2\pi\hbar} \int\limits_0^{\infty} \frac{d\varepsilon}{\sqrt{\varepsilon}}\ \Gamma(\varepsilon)|\varphi_\varepsilon(x)|^2. \tag{16}$$

Here the eigenfunctions of the continuous spectrum are normalized by the asymptotics at $x \to \infty$:

$$\langle|\varphi_\varepsilon^2|\rangle \overset{x\to\infty}{\longrightarrow} 1, \tag{17}$$

where $\langle\rangle$ denotes averaging over the period of the wave functions oscillations (18).

Now we can insert here the quasi–classical approximation [2] for the solution of the equation (4) which fulfills the zero boundary condition on the surface:

$$\varphi_\varepsilon^{wkb}(x) = \sqrt{2}\ \frac{(2m_e^*\varepsilon)^{1/4}}{\sqrt{p_\varepsilon(x)}} \sin\left(\frac{1}{\hbar}\int\limits_0^x p_\varepsilon(x')dx'\right), \tag{18}$$

$$p_\varepsilon(x) = \sqrt{2m_e^*\left(\varepsilon - qV(x) - qU(x)\right)}.$$

We see, that the charge density has to be found from the solution of the system, consisting of the one-body Schrd̈inger equation, the Poisson equation and the electroneutrality condition. This system is highly nolinear. Usually the solution of it is constructed by the sequence of the selfconsistant calculations, as described above.

Using the above-mentioned relations one can calculate the total charge (Q) and differential capacity (C) of the 2D-accumulation layer:

$$Q = \int\limits_0^{\infty}[\rho_e(x) + \rho_h(x)]dx = \int\limits_0^{\infty}[\rho_c^{wkb}(x) + \rho_q(x) + \rho_h(x)]dx = Q^{wkb} + Q_q + Q_p, \tag{19}$$

$$C = \frac{d\,Q}{dV_s} = C^{wkb} + \sum_i C_i + C_h = C^{wkb} + C_q + C_h \tag{20}$$

where C^{wkb}, C_i, C_h are the contributions, in the capacitance of the electrons in the continuous spectrum on the i-band states and holes, respectively.

3 Methods of calculation and numerical methods.

We rewrite the Schrödinger (4) and Poisson (6) equations in dimensionless variables:

$$\frac{d^2\,v(\tilde{x})}{d\,\tilde{x}^2} = -\left[(\rho_e^{wkb}(\tilde{x}) + \rho_q(\tilde{x}))/q - N_v(\tilde{x})F_{1/2}(-\varepsilon_f - \varepsilon_g - v_s(\tilde{x}))\right]/(n_0 + p_0), \tag{21}$$

$$\frac{d^2\,\varphi(\tilde{x})}{d\,\tilde{x}^2} + \frac{2m_e^* L_D^2 kT}{\hbar^2}\,(\varepsilon + v(\tilde{x}))\varphi(\tilde{x}) = 0, \tag{22}$$

here $\varepsilon = E/(kT)$ is the dimensionless energy, $v = q\frac{U+V}{kT}$ is the dimensionless potential, n_0, p_0 are the equilibrium concentrations of electrons and holes in the space respectively, $\tilde{x} = x/L_D$ is the length normed to the Debye length $L_D = \sqrt{\varepsilon_0 \varepsilon_{sc} kT/(q^2(n_0+p_0)}$, and the normalization of the wave function is choosen as

$$\int_0^\infty |\varphi(\tilde{x})|^2 \, d\tilde{x} = 1/L_D.$$

All dimensionless constants are chosen so that the real properties of antimonid Indium are taken into account.

The wave function of electrons in the continuum is represented by WKB approximation:

$$\varphi_\varepsilon^{wkb}(\tilde{x}) = \sqrt{2} \, \left(\frac{\varepsilon}{\varepsilon + v(\tilde{x})}\right)^{1/4} \sin\left(\frac{\sqrt{2\pi m_e^* kT} L_D}{\hbar} \int\limits_0^{\tilde{x}} \sqrt{\varepsilon + v(\tilde{x}')} d\tilde{x}'\right).$$

In what follows we omit the bar over x, but sill keep in mind, that x is a dimensionless variable. The equations (21) and (22) are connected via $v(x)$, ε, $\varphi(x)$ and are solved in traditional self-consistent way [1]. The iterative procedure of the self-consistent solution of the Poisson and Schrödinger equations is formed in the following way. As an initial input potential $v_{in}^1(x) \equiv U(x)$ in (22), we substitute the solution of the Poisson equation in (26) for the classical case and find the values ε_n, the wave functions $\varphi_n(x)$, the populations Γ_n and, as a final result, the charge density of electrons in the discrete spectrum $\rho_q(x)$. Further we calculate the charge density in the continuum $\rho_c^{wkb}(x)$. Now solving the right side of the Poisson equation, we determine a new additional potential in the semiconductor space $v_{out}^1(x)$. The condition of electroneutrality is used to calculate the Fermi lavel of the semiconductor.

For the following iterations we set the next effective input potential

$$v_{in}^{k+1}(x) = \alpha v_{out}^k(x) + (1-\alpha) v_{in}^k(x).$$

The coefficient is selected the $\alpha = 0.5$ [1]. The iterative process is taken for completed when

$$\max_{x_j,\ j=\overline{0,N-1}} |v_{out}^k - v_{in}^k| < 10^{-5}.$$

The Poisson equation are solved by the grid method. We choose the grid as $\omega = \{x_j = j\Delta l,\ j = \overline{0, N-1}\}$ (N is equal to 2048, and $l = 50$). The grid approximation (6) is formed as follows:

$$\frac{v(x_{j-1}) - 2v(x_j) + v(x_{j+1})}{\Delta l^2} = -\frac{\left[(\rho_e^{wkb}(x_j) + \rho_q(x_j))/q - N_v(x_j) F_{1/2}(-\varepsilon_f - \varepsilon_g - v_s)\right]}{(n_0 + p_0)} \tag{23}$$

with the boundary conditions $v(x_0) = v_s,\ v(x_{N-1}) = 0$. This system of nonlinear algebraic equations is solved by the iterative method with respect to the three-layer implicit scheme [6]. The accuracy of the solution (23) is not worse than 10^{-10}.

The Schrödinger equation (22) is solved on each step by finite-difference method, the second derivative is represented by the three-point scheme ($\varphi(x_j) = \varphi_j$)

$$\frac{d^2\varphi}{dx^2}|_{x=x_j} = \frac{\varphi_{j-1} - 2\varphi_j + \varphi_{j+1}}{\Delta l^2}.$$

This way the equation (22) is reduced to the linear algebraic equations system:

$$\varphi_{j-1} - 2\varphi_j + \varphi_{j+1} + D(\varepsilon_n + v(x_j)\varphi_j = 0, \tag{24}$$
$$\varphi_0 = 0, \qquad \varphi_N = 0, \qquad j = 1, 2, \ldots, N,$$
$$D = \frac{2m_e^* L_D^2 \Delta l^2 kT}{\hbar^2} \qquad ,$$

which is described by the symmetrical three-diagonal matrix:

$$\begin{bmatrix} -(2+Dv(x_1)) & 1 & 0 \ldots 0 & 0 \\ 1 & -(2+Dv(x_2)) & 1 \ldots 0 & 0 \\ \ldots & \ldots & \ldots\ldots\ldots & \ldots \\ 0 & 0 & 0 \ldots 1 & -(2+Dv(x_{N-2})) \end{bmatrix} \times \begin{bmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \\ \varphi_{N-2} \end{bmatrix} = D\varepsilon \begin{bmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \\ \varphi_{N-2} \end{bmatrix}$$

or

$$A\vec{\varphi} = \varepsilon D\vec{\varphi}. \tag{25}$$

Thus we've reduced the original problem to the problem of the construction of the eigenvalues and eigenfunctions [7].

For calculating ρ_e^{wkb} the numerical integration [7] is produced twice. The integral in (18) is calculated by the Sympson rule, and the integral in (16) is computed by the midpoint rule with the change of variable $\tau = -\ln t$, since the integral function decreases exponentially:

$$\int_{\tau=a}^{\tau=\infty} f(\tau)\, d\tau = \int_{t=0}^{t=\exp(-a)} f(-\ln t)/t\, dt.$$

4 Results of calculations.

The comparison of spectra of bound states obtained by the traditional Fermi and quasi–classical description of the continuum is represented in Fig.1. One can see from the Figure that for any of two selected values of the exterior ("surface") potential the position of quantum subbands are distinguished with respect to energies and their number. The presence of larger number of bound states and their deepening when using the WKB–description in comparison with the traditional one is caused by the effective broadening of the potential well. This broadening is a natural result of the assumption that the wave function of electrons in the continuum has a knot at the surface of semiconductor.

Figs.2 and 3 show the dependence of electrostatic potential in the semiconductor space,the energy levels of quantum subbands, the position of the Fermi level and wave functions of bound states for two values of the surface potential. It appeares,that the distance between the first and second quantum subbands *exceed the value of the thermal fuzzifying (kT=0.025 eV) for the narrow–gap semiconductor InSb at room temperature* .

Fig.4 represents distributions of electron densities on quantum subbands (1) in the continuous spectrum (2) and the total density (3). As usual [5], the step-wise singularities are present on the curve 1. These steps reveal singularities of charge distribution and localization in the quantum subbands. We can see from the curve 2 that the charge density of electrons in the continuum is minimal just over the potential well and tends to the equilibrium value of the concentration of electrons at infinity inside of the semiconductor.

The number of the peaks of charge density disposed over the potential seems to be equal to the number of bound states inside the well, and their amplitudes and the period of oscillations decrease with growing x. The correlated behaviour of charge density "over" the potential well and "inside" of it (in a sence of corresponding values of energy) testifies on a smooth dependence of the total charge density of electrons in the two-dimensional accumulation layer on coordinates.

The calculation of energy dependence of quantum subbands at $T = 300\,\mathrm{K}$ is presented in Fig.5. As it is seen from the Figure, the number of bound states growths when the value of surface potential is growing . It is caused by the deepening and broadening of the potential well. One can determine the range of change V_s, in which the distance between the first and second subbands is greater then kT.

The dependence of the number of levels and their positions on temperature for the fixed value of surface potential is shown in Fig.6. It is seen that, when decreasing temperature, the number of states in the potential well increases (first six levels are indicated only). One can see, that the number of energy levels in the potential well is growing when decreasing temperature. It is possible caused by the decreasing of the screening depth at low temperatures, when the number of free charge carriers is relatively small. Thus the effective width of the potential well increases and the number of the energy levels inside of it increases as well. Practically it might impede spectroscopic distinguishing them. *Surprisingly these levels will be more easily observed for higher temperatures.*

The conclusion is found to be paradoxical, namely, the raised (room) temperatures prove to be more preferable for observing of bound states in the narrow-gap semiconductor. It is known that for observing quantum effects on the surface of semiconductor the following conditions are necessary:

— the number of bound states has to be minimal;

— the distance between quantum subbands exceeds the value of thermal fuzzifying (kT) and collisional broadening.

Indeed, in our case at room temperature $T \sim 300\,\mathrm{K}$ the number of bound states in the potential well is minimal (Fig.6) and the distance between them exceeds the value of thermal fuzzifying. Moreover, the collisional broadening of quantum subbands is very small due to *high mobility of electrons in antimonid indium.*

The dependence of the total charge in the 2D-accumulation layer Q (curve 1) and the total charge of electrons in quantum subbands Q_q (curve 2) on the surface potential and temperature, respectively, (see, formula (19)) is represented in Figs.7 and 8. One can see from the Figures (curve 1) that the total charge growths monotonically with increasing surface potential and temperature. At the same time the charge variation in quantum subbands is growing in step-wise fashion. We can see from the Fig.7 that this step-wise growing with growth of surface potential is correlated with the birth of new discrete levels from the continuum and their occupation.

The dependence of charge in quantum subbands on temperature (Fig.6, curve 2) has a specific form. Peaks at the curve 2 are connected with moments of transition of levels from the discrete spectrum in the potential well to the continuous one over the well with growing temperature.

The dependence of the total differential capacitance (C) and the contribution to it of charge carriers in bound states (C_i) and in the continuum (C^{wkb}) on surface potential are represented in Fig.9. The similar dependence of differential capacitance C^{cls} calculated for accumulation layers InSb with no account of the dimensional quantization are shown to compare with. The value of the surface potential in which the new levels appear, is marked by gray bands in the Figure. The correct calculation of capacitance at these potentials is extremely difficult because of instability of the computations at these places.

The nontrivial behaviour of the capacitance near the potential of plane bands should be noticed. Its decreasing up to the moment of birth of the second quantum subband C_2 is correlated with sharp dropping C^{wkb} at weak variation of charge at the first quantum level (see Fig.7, curve 2). Decreasing of total capacitance can be explained by the fact that the centroid of total charge is always smaller (see Fig.10) for quantum description than for classical one (without dimensional quantization)

5 Conclusion.

In frames of the present work the following results were obtained:

- the mathematical model of the 2D system based on the InSb surface was developed for accumulation layers;
- the calculation of the 2D system parameters was carried out by numerical self-consistent integration of the Schrödinger and Poisson equations by using the Fermi and quasi-classical (WKB) descriptions of the continuum of electrons;
- it was shown that the quasi-classical approximation is more preferable in comparison with the Fermi one for the selfconsistant calculations of electron density in the states of continuous spectrum;

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Subscript to Figures.

Fig.1. Spectra of bound states at the Fermi and quasi-classical description of the continuous spectrum.

Fig.2. Behaviour of electrostatical potential and energies of quantum subbands.

Fig.3. Wave functions of bound states.

Fig.4. Distribution of electron charge density: *1* — in the continuous spectrum; *2* — in the discrete spectrum; *3* — total electron charge density.

Fig.5. Dependence of position of quantum subbands on surface potential.

Fig.6. Dependence of position of quantum subbands on temperature.

Fig.7. Dependence of charge in the 2D-layer on surface potential: *1* — total charge; *2* — charge in subbands.

Fig.8. Dependence of charge in the 2D-layer on temperature: *1* — total charge; *2* — charge in subbands.

Fig.9. Dependence of differential capacitance of the 2D-layer on surface potential.

Fig.10. Dependence of charge centroid on surface potential: Fermi (1) and quasi–classical (2) description of charge in the continuum spectrum.