APPLICATION OF HOMOTOPY PERTURBATION METHOD IN SOLVING COUPLED SCHRÖDINGER AND POISSON EQUATION IN ACCUMULATION LAYER

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Abstract. In this manuscript, a novel approach for an approximate solving of coupled Schrödinger-Poisson (SP) equations in the accumulation layer of semiconductor is described. This approach, based on the homotopy perturbation method (HPM), gives an approximate analytic solution of SP system which at the same time has a relative simple mathematical form, as well as a high degree of accuracy. A good agreement between HPM solution and exact solution of SP system indicates on the utility and sufficiency of the HP method.

Key words: Homotopy perturbation, coupled SP equations, accumulation layer, approximation.

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1. INTRODUCTION

Application of an electric field normal to the surface of a semiconductor attracts the majority charge carriers in the semiconductor to the surface. As a result of this redistribution of charge carriers an accumulation layer is created at the surface, causing a band bending there. Width of the resulting potential well in direction perpendicular to the surface is small compared to the wavelengths of the carriers [1]. Thus the energy level of the carriers are grouped in subbands, each of which corresponds to a quantized level in direction perpendicular to the surface with a continuum for motion in the plane parallel to the surface [2].

Besides the carriers confined in potential well, there are also the free carriers whose motion perpendicular to the surface is not quantized and whose wave functions extend as traveling waves into the bulk. These carriers form the space charge in the bulk compensating for the charge of the ionized impurities. Near the surface the

traveling waves are distorted by the varying potential and these carriers also make a contribution to the space charge in the accumulation layer. However, in the case of a non-degenerate semiconductor at the sufficiently low temperature the number of ionized impurities is negligible what greatly reduces the complexity of the problem. Furthermore, the most of the carriers occupy only the lowest energy level, *i.e.* we have a situation known as the electric quantum limit [3]. The motion of the carriers in the accumulation layer is described by Schrödinger wave equation while their charge distribution must satisfy the Poisson equation [4]. Thus, Schrödinger and Poisson (SP) equations are coupled here, and these need to be solved simultaneously and self-consistently in order to find the carrier concentration present in the accumulation layer. Unfortunately, the SP system can be solved only numerically with no the analytical expression which would give the insight into overall behavior of the obtained solutions. On the other hand, since the accumulation layer is critical to the performance of many solid state devices, such as microelectronics, optoelectronics, sensors and solar cells, from a circuit modeling point of view, analytical solution of the SP system is desirable [5]. Due to this reason some approximate methods for analytical solving of SP system have been made and provided satisfactory results in some specifically cases [6–8] or for the finite interval [3].

In order to solve the SP system along the whole semiconductor, *i.e.* along the infinite interval, here we propose the application of the homotopy perturbation method (HPM). The HPM proposed by He [9]-[12], is a general approach used to obtain (approximate) solutions of the non-linear equations of various types. Different from all other analytic methods, it provides a simple way to adjust and control the convergence region of solution series by choosing proper values for auxiliary parameters (functions). This method has been the subject of extensive studies in the recent years [13]-[15], and it was applied to solving the different kinds of problems, mainly in the physical sciences [16]-[19]. Especially, the HPM has been used in solving the non-linear Schrödinger equation of various kinds [20, 21]. On the other side, Poisson equation has been mainly solved by different, mostly numerical approximate methods [22] or by applying the so-called Homotopy Analysis Method (HAM) [23].

2. DEFINITION OF THE PROBLEM

We consider an accumulation layer on the surface of n-type semiconductor. Under the assumption that the effective-mass approximation is valid, we can neglect the periodic potential and use the effective masses and the dielectric constant of the perfect crystal. In the electric quantum limit the coupled set of Schrödinger and

Poisson equation has following form:

$$-\frac{\hbar^2}{2m_z}\frac{\mathrm{d}^2\xi(z)}{\mathrm{d}z^2} - qV(z)\xi(z) = E_0\xi(z), \tag{1a}$$

$$\frac{\mathrm{d}^2V(z)}{\mathrm{d}z^2} = \frac{qN_0}{\varepsilon_s}|\xi(z)|^2. \tag{1b}$$

Here, $\xi(z)$ is the normalized wave function for the lowest energy level E_0, ε_s is the dielectric constant of the semiconductor, $V(z)$ and N_0 is the potential and the total number of electrons in the accumulation layer, respectively.

The set of equations independent of the particular semiconductor under study can be obtained by introducing the following set of dimensionless variables:

$$x = z\left(\frac{q^2\,m_z\,N_0}{\varepsilon_s\,\hbar^2}\right)^{1/3}, \quad \phi(x) = V(z)\left(\frac{\varepsilon_s^2\,m_z}{q\,\hbar^2\,N_0^2}\right)^{1/3},$$

$$\varepsilon_0 = E_0\left(\frac{\varepsilon_s^2\,m_z}{q^4\hbar^2N_0^2}\right)^{1/3}, \quad \psi(x) = \xi(z)\left(\frac{\varepsilon_s\,\hbar^2}{q^2\,m_z\,N_0}\right)^{1/6}. \tag{2}$$

With these equations, we get the following set of dimensionless equations for an accumulation layer at the electric quantum limit:

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + 2\left(\phi(x) + \varepsilon_0\right)\psi(x) = 0 \tag{3a}$$

$$\frac{\mathrm{d}^2\phi(x)}{\mathrm{d}x^2} - \psi^2(x) = 0, \tag{3b}$$

with boundary conditions:

$$\psi(x) = 0, \quad \text{when} \quad x = 0 \quad \text{and} \quad x \to \infty,$$

$$\phi(x) = \frac{\mathrm{d}\,\phi(x)}{\mathrm{d}x} = 0, \quad \text{when} \quad x \to \infty. \tag{4}$$

Further, the wave function must obey the normalization condition:

$$\int_0^\infty |\psi(x)|^2\,\mathrm{d}x = 1.$$

In general, the analytical solution of the coupled system of Eqs.(3a)-(3b) is not possible. Here, the new method based on the homotopy perturbations will be applied for approximate solving of this system of SP equations.

3. HPM APPROXIMATIONS OF THE COUPLED SP-EQUATIONS

To solve the coupled Eqs.(3a)-(3b) with the boundary conditions (4), we construct the following *homotopy equations*:

$$(1-p)\left[\frac{\partial^2 \Psi(x;p)}{\partial x^2} - \frac{\mathrm{d}^2\psi_0(x)}{\mathrm{d}x^2}\right] + p\,h_1\left[\frac{\partial^2 \Psi(x;p)}{\partial x^2} + 2\left(\Phi(x;p)+\varepsilon_0\right)\Psi(x;p)\right] = 0 \tag{5a}$$

$$(1-p)\left[\frac{\partial^2 \Phi(x;p)}{\partial x^2} - \frac{\mathrm{d}^2\phi_0(x)}{\mathrm{d}x^2}\right] + p\,h_2\left[\frac{\partial^2 \Phi(x;p)}{\partial x^2} - \Psi^2(x;p)\right] = 0. \tag{5b}$$

Here, $p \in (0,1)$ is *the embedding parameter*, and $h_1, h_2 : [0,\infty) \to [0,1]$ are *the auxiliary functions*. For $p = 0$, the homotopy Eqs.(5a)-(5b) have the so-called *initial solutions (approximations)*:

$$\Psi(x;0) = \psi_0(x) \quad \text{and} \quad \Phi(x;0) = \phi_0(x).$$

The initial solutions $\psi_0(x)$ and $\phi_0(x)$ can be chosen arbitrarily, but such to meet boundary conditions $\psi_0(0) = \psi_0(\infty) = 0$, and $\phi_0(\infty) = \mathrm{d}\phi_0(\infty)/\mathrm{d}x = 0$. Similarly, when $p = 1$, Eqs.(5a)-(5b) become equivalent to original Eqs.(3a)-(3b), with the same boundary conditions.

The basic assumption of the HPM is that solutions of homotopy Eqs.(5a)-(5b) can be expressed as the power series in p:

$$\Psi(x;p) = \sum_{j=0}^{\infty} p^j\,\psi_j(x), \quad \Phi(x;p) = \sum_{k=0}^{\infty} p^k\,\phi_k(x). \tag{6}$$

According to Eqs.(5a)-(5b) and Eq.(4), solutions of the coupled SP-equations, given by Eqs.(1a)-(1b), can be obtain as:

$$\psi(x) = \lim_{p \to 1^-}\Psi(x;p) = \sum_{j=0}^{\infty}\psi_j(x), \tag{7a}$$

$$\phi(x) = \lim_{p \to 1^-}\Phi(x;p) = \sum_{k=0}^{\infty}\phi_k(x). \tag{7b}$$

In doing so, it is necessary that the both of series in Eqs.(7a)-(7b) converge. Substituting the power series defined by Eq.(6) in homotopy Eqs.(5a)-(5b), and by rearranging

some terms, the following equations are valid:

$$\sum_{j=1}^{\infty} p^j \frac{\mathrm{d}^2 \psi_j(x)}{\mathrm{d}x^2} + (h_1(x) - 1) \sum_{j=1}^{\infty} p^j \frac{\mathrm{d}^2 \psi_{j-1}(x)}{\mathrm{d}x^2} + p \frac{\mathrm{d}^2 \psi_0(x)}{\mathrm{d}x^2}$$

$$+ 2h_1(x) \left[p \Big(\sum_{j=0}^{\infty} p^j \psi_j(x) \Big) \Big(\sum_{k=0}^{\infty} p^k \phi_k(x) \Big) + \varepsilon_0 \sum_{j=1}^{\infty} p^j \psi_{j-1}(x) \right] = 0, \quad (8a)$$

$$\sum_{k=1}^{\infty} p^k \frac{\mathrm{d}^2 \phi_k(x)}{\mathrm{d}x^2} + (h_2(x) - 1) \sum_{k=1}^{\infty} p^k \frac{\mathrm{d}^2 \phi_{k-1}(x)}{\mathrm{d}x^2}$$

$$+ p \frac{\mathrm{d}^2 \phi_0(x)}{\mathrm{d}x^2} - p\, h_2(x) \left(\sum_{j=0}^{\infty} p^j \psi_j(x) \right)^2 = 0. \quad (8b)$$

Equating in Eqs.(8a)-(8b) expressions with the identical powers p^j, p^k, $j, k = 1, 2, \ldots$, we obtain the following differential equations:

$$\begin{cases} \dfrac{\mathrm{d}^2 \psi_1(x)}{\mathrm{d}x^2} + h_1(x) \left[\dfrac{\mathrm{d}^2 \psi_0(x)}{\mathrm{d}x^2} + 2\big(\phi_0(x) + \varepsilon_0\big) \psi_0(x) \right] = 0 \\ \dfrac{\mathrm{d}^2 \phi_1(x)}{\mathrm{d}x^2} + h_2(x) \left[\dfrac{\mathrm{d}^2 \phi_0(x)}{\mathrm{d}x^2} - \psi_0^2(x) \right] = 0, \end{cases} \quad (9)$$

and, for $k \geq 2$:

$$\begin{cases} \dfrac{\mathrm{d}^2 \psi_k(x)}{\mathrm{d}x^2} = (1 - h_1(x)) \dfrac{\mathrm{d}^2 \psi_{k-1}(x)}{\mathrm{d}x^2} - 2h_1(x) \left[\displaystyle\sum_{j=0}^{k-1} \psi_j(x)\phi_{k-j-1}(x) + \varepsilon_0\, \psi_{k-1}(x) \right] \\ \dfrac{\mathrm{d}^2 \phi_k(x)}{\mathrm{d}x^2} = (1 - h_2(x)) \dfrac{\mathrm{d}^2 \phi_{k-1}(x)}{\mathrm{d}x^2} + h_2(x) \displaystyle\sum_{j=0}^{k-1} \psi_j(x)\psi_{k-j-1}(x). \end{cases}$$

$$(10)$$

In addition, we suppose that the same boundary conditions $\psi_j(0) = \psi_j(\infty) = 0$ and $\phi_k(\infty) = \mathrm{d}\phi_k(\infty)/\mathrm{d}x = 0$ hold. In this way, Eqs.(9)-(10) can be solved recursively on $\psi_j(x)$, $\phi_k(x)$ for each $j, k = 1, 2, \ldots$, using the double integration on $(0, +\infty)$. According to these, *the HPM-approximations* of unknown functions $\psi_($x$)$ and $\phi_($x$)$, for any $k = 0, 1, 2, \ldots$ will be, respectively:

$$\widehat{\psi}_k(x) := \sum_{j=0}^{k} \psi_j(x), \qquad \widehat{\phi}_k(x) := \sum_{j=0}^{k} \phi_j(x), \quad (11)$$

where the normalized condition $\int_0^{\infty} \left| \widehat{\psi}_k(x) \right|^2 \mathrm{d}x = 1$ holds. In the following, the

existence and convergence of these approximations, under the certain necessary conditions, will be researched more precisely.

Theorem 1 Let $\{\psi_k(x)\}_{k=0}^{\infty}$ and $\{\phi_k(x)\}_{k=0}^{\infty}$ be the sequences of continuous functions, defined on $(0, \infty)$ by recurrence relations in Eqs.(9)–(10). Let assume that the sequences $\{\psi_k(x)\}_{k=0}^{\infty}$, as well as the function $\phi_0(x)$, are uniformly bounded and exponentially decrease, *i.e.*, for some $M_1, M_2 > 0$ the inequalities

$$|\psi_k(x)| \leq M_1 \exp\left(-(k+1)x\right), \quad |\phi_0(x)| \leq M_2 \exp(-x), \qquad (12)$$

hold for any $k = 0, 1, 2\ldots$, and for all $x \in (0, \infty)$. Then, the sequences $\{\widehat{\psi}_k(x)\}_{k=0}^{\infty}$ and $\{\widehat{\phi}_k(x)\}_{k=0}^{\infty}$, defined by Eq.(11), converge on $(0, \infty)$. Furthermore, their limits are given by Eqs.(7a)–(7b), and they are solutions of the Eqs.(3a)–(3b), respectively.

Proof. Denote $M = \max\{M_1, M_2\}$, and for an arbitrary but fixed $x \geq 0$, let $r_1(x)$ and $r_2(x)$ be the radius of convergence of the power series in Eq.(6), respectively. Thus, according to assumptions of the theorem, *i.e.*, the first inequality in (12), for each $k = 0, 1, 2, \ldots$ we have:

$$|\psi_k(x)|^{1/k} \leq M^{1/k} \exp\left(-x - 1/k\right).$$

In addition, by using second equations in Eqs.(9)-(10), for the sequence $\{\phi_k(x)\}$ we have:

$$|\phi_1(x)| \leq h_2(x) \left[|\phi_0(x)| + \int \mathrm{d}x \int |\psi_0(x)|^2 \mathrm{d}x \right]$$

$$\leq M h_2(x)\, \mathrm{e}^{-x} + M^2 h_2(x)\, \mathrm{e}^{-2x} \qquad (13)$$

and, when $k \geq 2$:

$$|\phi_k(x)| \leq (1 - h_2(x)) |\phi_{k-1}(x)| + h_2(x) \int \mathrm{d}x \int \sum_{j=0}^{k-1} |\psi_j(x)| |\psi_{k-j-1}(x)| \,\mathrm{d}x$$

$$\leq (1 - h_2(x)) |\phi_{k-1}(x)| + M^2 h_2(x) \sum_{j=0}^{k-1} \int \mathrm{d}x \int \mathrm{e}^{-(j+1)x} \mathrm{e}^{-(k-j)x} \mathrm{d}x$$

$$\leq (1 - h_2(x)) |\phi_{k-1}(x)| + h_2(x) \frac{k M^2 \exp\left(-(k+1)x\right)}{(k+1)^2}$$

$$\leq (1 - h_2(x)) |\phi_{k-1}(x)| + M^2 h_2(x) \exp\left(-(k+1)x\right). \qquad (14)$$

Applying Cauchy-Hadamard theorem, we find that:

$$r_1(x) = \left[\limsup_{k\to\infty} |\psi_k(x)|^{1/k} \right]^{-1} \geq \lim_{k\to\infty} \left[M^{-1/k} \exp\left(x + 1/k\right) \right] = \exp(x) \geq 1,$$

$$r_2(x) = \left[\limsup_{k\to\infty} |\phi_k(x)|^{1/k} \right]^{-1} \geq \lim_{k\to\infty} \left[|\phi_{k-1}(x)| + M^2 \exp\left(-(k+1)x\right) \right]^{-\frac{1}{k}} = 1,$$

i.e. the radius of convergence of both series defined in Eq.(4) is not smaller than 1.

On the other hand, applying the induction method in (11)-(12) and after some computations, it follows that for an arbitrary $k \geq 1$:

$$|\phi_k(x)| \leq M h_2(x)(1 - h_2(x))^{k-1} \mathrm{e}^{-x} + M^2 h_2(x) \sum_{j=1}^{k} \mathrm{e}^{-(j+1)x}(1 - h_2(x))^{k-j}$$

$$\leq \mathrm{e}^{-x} \left[M(1 - h_2(x))^{k-1} + M^2 h_2(x) \frac{(1 - h_2(x))^k - \mathrm{e}^{-kx}}{(1 - h_2(x))\mathrm{e}^x - 1} \right].$$

Now, according to the definition of HPM approximations $\widehat{\psi}(x)$ and $\widehat{\phi}(x)$, given by Eq.(11), we obtain for each $k \geq 0$:

$$\left| \widehat{\psi}_k(x) \right| \leq M \sum_{j=0}^{k} \mathrm{e}^{-(j+1)x},$$

as well as for $k \geq 1$:

$$\left| \widehat{\phi}_k(x) \right| \leq M \mathrm{e}^{-x} \left[1 + h_2(x) \sum_{j=1}^{k} (1 - h_2(x))^{j-1} + M h_2(x) \sum_{j=1}^{k} \frac{(1 - h_2(x))^j - \mathrm{e}^{-jx}}{(1 - h_2(x))\mathrm{e}^x - 1} \right].$$

Under conditions $x > 0$ and $h_2(x) \neq 0$, the inequalities above imply, when $k \to \infty$:

$$\left| \sum_{j=0}^{\infty} \psi_j(x) \right| = \lim_{k \to \infty} \left| \widehat{\psi}_k(x) \right| \leq \frac{M}{\mathrm{e}^x - 1} < +\infty,$$

$$\left| \sum_{j=0}^{\infty} \phi_j(x) \right| = \lim_{k \to \infty} \left| \widehat{\phi}_k(x) \right| \leq 2M\mathrm{e}^{-x} + \frac{M^2 \mathrm{e}^{-x}}{\mathrm{e}^x - 1} < +\infty.$$

In this way, sequences $\{\widehat{\psi}_k(x)\}_{k=0}^{\infty}$ and $\{\widehat{\phi}_k(x)\}_{k=0}^{\infty}$, *i.e.*, series $\sum_{j=0}^{\infty} \psi_j(x)$ and $\sum_{j=0}^{\infty} \phi_j(x)$ converge on $(0, \infty)$.

Finally, according to Abel's theorem (see, for instance [24]), it follows that functions $\widetilde{\Psi}(x, p)$ and $\widetilde{\Phi}(x, p)$, defined by Eq.(4), are continuous from the left at $p = 1$. Therefore, Eqs.(7a)–(7b) hold, *i.e.*, series $\sum_{j=0}^{\infty} \psi_j(x)$ and $\sum_{j=0}^{\infty} \phi_j(x)$ are solutions of Eqs.(3a)–(3b), respectively. $\square$

Remark 1 Thanks to the appropriate choices of the electronic wave function and the electrostatic potential, the conditions of the previous theorem are usually fulfilled in solving of the accumulation layer problem. In the following, a practical interpretation (and validation) of all these conditions will be seen.

4. VALIDATION OF THE HPM PROCEDURE

The primary question in practical application of the aforementioned HPM procedure is choice of initial solutions, which will ensure a convergence of the HPM-approximations, defined by Eqs.(9). Additionally, these solutions must also satisfy the boundary conditions in Eq.(2), and should be simple for integration. Due to these reasons, as the initial solution of Schrödinger equation we have taken the function:

$$\psi_0(x) = W_{k,m}(2x),$$

where $W_{k,m}(x)$ is the Whittaker function of the second kind, *i.e.*,

$$W_{k,m}(x) := e^{-\frac{x}{2}} x^{m+\frac{1}{2}} U\left(\frac{1}{2} + m - k; 2m + 1; x\right)$$

and

$$U(a,b;x) := \frac{1}{\Gamma(a)} \int_0^\infty \mathrm{e}^{-xt} t^{a-1} (1+t)^{b-a-1} \mathrm{d}t$$

is the confluent hypergeometric function. More specifically, we have taken $k = 1$ and $m = 1/2$, so the condition $\psi_0(0) = \psi_0(\infty) = 0$, as well as the normalization condition $\int_0^\infty |\psi_0|^2 \, \mathrm{d}x = 1$ is fulfilled.

After that, we have computed HPM-approximations with two specific choices of initial solutions $\phi_0(x)$ of electrostatic potential:

1. The first series of HPM-approximations has based on the trivial initial solution for the potential $\phi(x)$, *i.e.* have taken $\phi_0(x) \equiv 0$.

2. The second HPM-approximations sequence has been obtained using the initial approximation for potential computed by immediate integration of Poisson's equation (1b):

$$\phi_0(x) = \int \mathrm{d}x \int h_2(x) |\psi_0(x)|^2 \, \mathrm{d}x = \frac{4}{27} \mathrm{e}^{-3x} \left(3x^2 + 4x + 2\right).$$

   Here, $h_2(x) = \exp(-x)$ is the auxiliary function which provides faster convergence of the sequence $\{\phi_k(x)\}$.

Thereafter, the others HPM-approximations can be obtained as the solutions of Eqs.(9)-(10). For the both of aforementioned series, labeled as A and B, respectively, the first few components are:

<u>Series A</u>:

$$\psi_1(x) = \frac{\mathrm{e}^{-2x}}{48}\left(-168x^2 + 119\mathrm{e}^x x - 288x + 204\mathrm{e}^x - 204\right),$$

$$\phi_1(x) = \frac{4}{27}\mathrm{e}^{-3x}\left(3x^2 + 4x + 2\right);$$

$$\psi_2(x) = \frac{e^{-5x}}{449776800000}\left(-31984128000x^4 + 7827189936\mathrm{e}^x x^3 + 1749132000000\mathrm{e}^{2x} x^3\right.$$

$$-93820108800x^3 + 22177038152\mathrm{e}^x x^2 + 5097470400000\mathrm{e}^{2x} x^2 - 4141985394960\mathrm{e}^{3x} x^2$$

$$-118554501120x^2 + 24459968550\mathrm{e}^x x + 6904906800000\mathrm{e}^{2x} x - 11185430790312\mathrm{e}^{3x} x$$

$$+2337580878129\mathrm{e}^{4x} x - 72326774784x + 9457854506\mathrm{e}^x + 3470500000000\mathrm{e}^{2x}$$

$$\left.-9563523115410\mathrm{e}^{3x} + 6103011610728\mathrm{e}^{4x} - 19446349824\right),$$

$$\phi_2(x) = \frac{e^{-4x}}{5184}\left(-4536x^3 + 8016\mathrm{e}^x x^2 - 15876x^2 + 20480\mathrm{e}^x x - 19683x\right.$$

$$\left.+11872\mathrm{e}^x - 7857\right); \quad \text{etc.}$$

<u>Series B</u>:

$$\psi_1(x) = \frac{\mathrm{e}^{-5x}}{135337500}\left(-9624000x^4 + 2675016\mathrm{e}^x x^3 - 28230400x^3 + 7579212\mathrm{e}^x x^2\right.$$

$$-473681250\mathrm{e}^{3x} x^2 - 35672960x^2 + 8359425\mathrm{e}^x x - 812025000\mathrm{e}^{3x} x + 337052016\mathrm{e}^{4x} x$$

$$\left.-21763072x + 3232311e^x - 575184375\mathrm{e}^{3x} + 577803456\mathrm{e}^{4x} - 5851392\right),$$

$$\phi_1(x) = \frac{1}{864}\mathrm{e}^{-4x}\left(384\mathrm{e}^x x^2 - 216x^2 + 512\mathrm{e}^x x - 216x + 256\mathrm{e}^x - 81\right); \quad \text{etc.}$$

In both cases, the auxiliary functions $h_1(x) = x\exp(-x)$ and $h_2(x) = \exp(-x)$ was used, as well as $\varepsilon_0 = 3$. The whole computation procedure has been implemented in the software package MATHEMATICA 11.0. In addition, we compute also *the maximum absolute errors*:

$$Err(\widehat{\psi}_k) := \max_{x\geq 0}\left|\frac{\mathrm{d}^2\widehat{\psi}(x)}{\mathrm{d}x^2} + 2\left(\widehat{\phi}(x) + \varepsilon_0\right)\widehat{\psi}(x)\right|,$$

$$Err(\widehat{\phi}_k) := \max_{x\geq 0}\left|\frac{\mathrm{d}^2\widehat{\phi}(x)}{\mathrm{d}x^2} - \widehat{\psi}^2(x)\right|,$$

as well as *the maximum iteration differences*:

$$\left\|\widehat{\psi}_k - \widehat{\psi}_{k-1}\right\| := \max_{x\geq 0}\left|\widehat{\psi}_k(x) - \widehat{\psi}_{k-1}(x)\right|,$$

$$\left\|\widehat{\phi}_k - \widehat{\phi}_{k-1}\right\| := \max_{x\geq 0}\left|\widehat{\phi}_k(x) - \widehat{\phi}_{k-1}(x)\right|,$$

which represent the measures of convergence in relation to the order of approximations. These values, obtained for the both of series of HPM-approximations, are given in following Tables 1–2.

Table 1

Maximum approximations errors, iteration differences and computational time of the HPM-approximations (Series A)

Approx. order (k)	$Err(\widehat{\psi}_k)$	$Err(\widehat{\phi}_k)$	$\left\|\widehat{\psi}_k - \widehat{\psi}_{k-1}\right\|$	$\left\|\widehat{\phi}_k - \widehat{\phi}_{k-1}\right\|$	CPU time (s)
1	0.89816	0.42121	0.14163	0.14548	0.093
2	0.32657	0.38199	0.10969	0.12875	0.109
3	0.09125	0.05666	0.02491	0.10336	0.156
4	0.02123	0.00196	0.01114	0.08571	0.297
5	0.00444	0.00039	0.00038	0.07818	0.500
6	0.00088	0.00001	0.00029	0.07490	1.296

Table 2

Maximum approximations errors, iteration differences and computational time of the HPM-approximations (Series B)

Approx. order (k)	$Err(\widehat{\psi}_k)$	$Err(\widehat{\phi}_k)$	$\left\|\widehat{\psi}_k - \widehat{\psi}_{k-1}\right\|$	$\left\|\widehat{\phi}_k - \widehat{\phi}_{k-1}\right\|$	CPU time (s)
1	0.89246	0.38337	0.14084	0.05270	0.094
2	0.32129	0.11149	0.10902	0.04287	0.219
3	0.08902	0.05666	0.02467	0.09068	0.578
4	0.02056	0.00035	0.00212	0.08724	1.438
5	0.00444	0.00034	0.00078	0.06471	1.485
6	0.00088	5.98(-6)	0.00037	0.02055	1.609

The usage of the HPM not only increases the accuracy of the approximations, but also reduces the computation time significantly compared to some numerical methods that can be found in the literature [25, 26]. Namely, the computation time (CPU) for each iteration is shown the last columns of Tables 1 and 1. As can be seen, in the case of A-series, HPM-approximations have a relative short computation time, in comparison to B-series. On the other hand, HPM-approximations $\{\widehat{\phi}_k(x)\}$ of the B-series converge somewhat faster, as a consequence of "closer" initial approximations $\phi_0(x)$. Convergences of the both series are shown also in Fig.1, where are plotted the HPM-approximations $\widehat{\psi}_k(x)$ and $\widehat{\phi}_k(x)$, when $k = 0, 1, 2, \ldots 6$.
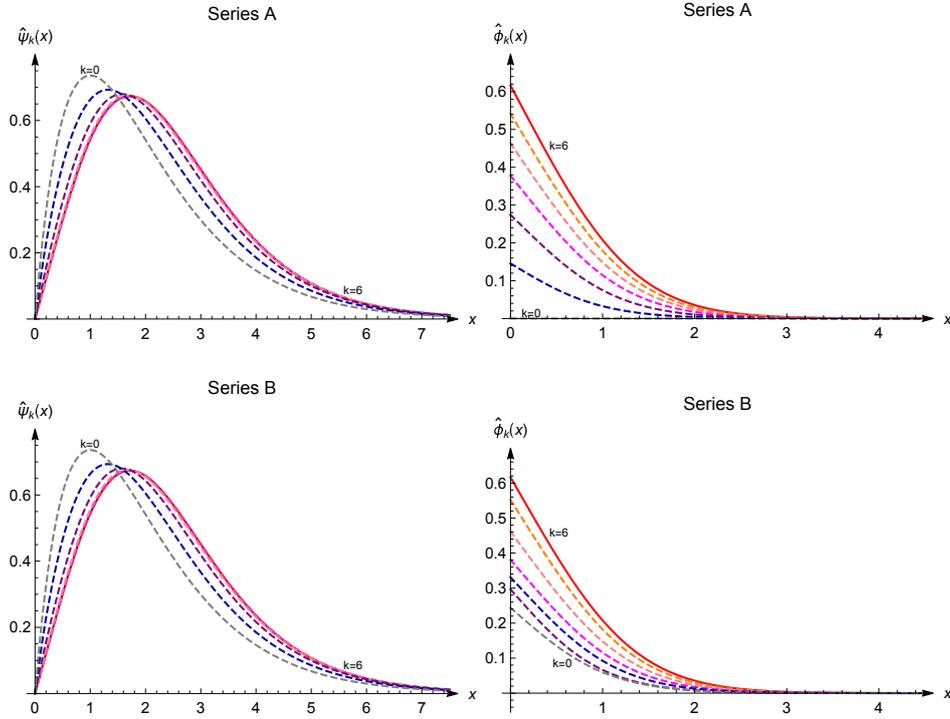
Fig. 1 – Graphs of the HPM-approximations $\widehat{\psi}_k(x)$ of the wave function $\psi(x)$ (panels left) and $\widehat{\phi}_k(x)$ of the potential $\phi(x)$ (panels right) with two different initial approximations: Series A (panels above) and Series B (panels bellow).

5. CONCLUSIONS

The accumulation layer problem in electric quantum limit is analyzed in this paper. The behavior of the electrons in the n-type accumulation layer, whose motion is quantized in direction perpendicular to the semiconductor's surface, is described by coupled system of SP equations. This system firstly has been simplified by introducing the appropriate dimensionless variables, and then the homotopy perturbation method has been applied for its solving. Results obtained using HPM converge to numerical solutions of SP-system along the entire convergence interval. Suitable agreement between obtained results and exact solution of SP system demonstrates the remarkable efficiency of the HPM. Moreover, the basic ideas of this approach can be also utilized to calculate the energy of the first allowed subband for electrons and the electron concentration in inversion layer of semiconductor. Furthermore, here proposed HPM could be easily extended on the case when more electric subbands are occupied by electrons.

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