

# Density Gradient Quantum Surface Potential

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## ABSTRACT

The PSP model [1], a generalized Surface-Potential (SP) model, has been chosen to be an industry standard for the next generation, 60nm, technology. In order to include quantum effects within surface potential models we use asymptotic analysis techniques [2], [3] applied to the the Density-Gradient equations [4]. Our quantum modified surface potential (SP) results from the ability to obtain a first integral of the Poisson equation.

**Keywords:** Surface Potential, Density Gradient, Quantum corrections, Asymptotic methods

## 1 The Quantum Problem

For MOSFETs, the ratio of the maximum channel dopant concentration to the intrinsic level is normally very large, therefore following [6], a large parameter  $\lambda$  is introduced as

$$\lambda = \max \left| \frac{N(x_1)}{n_i} \right| = \frac{N_A}{n_i},$$

where  $N_A$  is the substrate doping and  $n_i$  is the intrinsic carrier density in silicon. To normalize the electron concentration in the device, the following rescaling is performed

$$(\psi, \Phi_n) = (w, \phi) V_{th} \ln \lambda, \quad x_1 = x L_D \left( \frac{2 \ln \lambda}{\lambda} \right)^{1/2}$$

where  $V_{th}$  is the thermal voltage,  $x_1$  is the coordinate perpendicular to the motion of carriers. The quantity  $L_D = \left( \frac{kT \epsilon_{si}}{n_i q^2} \right)^{1/2}$  is the Debye length.

In the DD model, the electron and hole drift potentials are  $\phi_n = \phi_p = \phi$ , but according to the DG model,  $\phi_n$  and  $\phi_p$  are given by

$$\begin{aligned} \phi_n &= \phi + \phi_{qn}, \quad \phi_{qn} = 2b_n \frac{\nabla^2 \sqrt{n}}{\sqrt{n}} \\ \phi_p &= \phi + \phi_{qp}, \quad \phi_{qp} = 2b_p \frac{\nabla^2 \sqrt{p}}{\sqrt{p}} \\ b_n &= \frac{\hbar^2}{4r_n m_n q}, \quad b_p = \frac{\hbar^2}{4r_p m_n q} \end{aligned}$$

where  $n$  and  $p$  are the electron and hole densities respectively,  $\hbar$  is Planck's constant,  $r$  is a fitting parameter,  $m$  is the mass of the electron and  $q$  is its charge. The quantum corrections  $\phi_{qn}$  and  $\phi_{qp}$  are derived from the Schrödinger equation, based on the finite curvature (energy) and strict continuity of wave functions.

In the DG model, a microscopic quantum description is used in regions with dominant quantum effects, and a macroscopic (fluid-type) model is employed in subregions where collisional effects are expected to be dominant [5]. In the expression for  $\phi_n$ , the correction  $\phi_{qn}$  to the quasi-Fermi potential is derived using Boltzmann statistics. With the quantum corrections to the DD model, the governing equations become

$$\frac{d^2 w}{dx^2} = \frac{n-p}{N_A} + 1, \quad (1a)$$

$$w - \phi = \frac{1}{\ln \lambda} \ln \left( \frac{n}{n_i} \right) - \frac{\lambda \beta^2}{(\ln \lambda)^2} \frac{1}{\sqrt{n}} \frac{d^2 \sqrt{n}}{dx^2}, \quad (1b)$$

where  $\beta^2 = \frac{2b_n}{V_{th} L_D^2}$ . The quantum correction does not affect the boundary conditions for the potential at the Si/SiO<sub>2</sub> interface, but using the well-accepted boundary condition for the electron density, the boundary conditions for (1) are  $n(0) = 0$ ,  $w(0) = w_s$ , and  $w(\infty) = w_\infty \sim -1$ , as well as the Robin boundary condition

$$\left. \frac{dw}{dx} \right|_{x=0} = c(w_s - V_{gs}), \quad (2)$$

## 2 The Subthreshold Case

The subthreshold case corresponds to the weak inversion regime, meaning  $0 \leq w_s(V_{gs}) \leq 1$ . In this case, the dominant contribution to the space charge density near the interface arises from the immobile acceptor ions,  $N_A$  [6]. Thus, the system of equations for the subthreshold case becomes

$$\frac{d^2 w}{dx^2} = 1, \quad (3a)$$

$$w - \phi = \frac{1}{\ln \lambda} \ln \left( \frac{n}{n_i} \right) - \frac{\lambda \beta^2}{(\ln \lambda)^2} \frac{1}{\sqrt{n}} \frac{d^2 \sqrt{n}}{dx^2}. \quad (3b)$$

We will determine the potential and electron density using matched asymptotic expansions (MAE's). This

is done by introducing a quantum inner layer near the interface governed by (3) and an outer depletion layer governed by the classical model, and properly matching them.

### 3 Asymptotics

In the region near the interface, the quantum inner layer, the device behavior is drastically different than in the classical case. Solutions in this layer are obtained by formal expansions in a small parameter,  $\varepsilon$ . Following [7], the quantum inner layer independent variable scaling is

$$X = \frac{x}{\varepsilon} \quad \text{where} \quad \varepsilon^2 = \frac{\lambda\beta^2}{2\ln\lambda}.$$

The dependent variables of (3) are also expanded formally in powers of  $\varepsilon$  as

$$(w, T, Y) = (W_0, T_0, Y_0) + \varepsilon(W_1, T_1, Y_1) + \mathcal{O}(\varepsilon^2),$$

where it is convenient, as in [7], to use the following rescaled variables

$$T = \sqrt{\frac{n}{n_i}} \quad \text{or} \quad Y = \frac{1}{\ln\lambda} \ln\left(\frac{n}{n_i}\right). \quad (4)$$

When the scaled independent variable  $X$  is substituted into (3a), the equation reads

$$\frac{d^2w}{dX^2} = \varepsilon^2 \quad \text{thus} \quad \frac{d^2}{dX^2}(W_0 + \varepsilon W_1 + \mathcal{O}(\varepsilon^2)) = \varepsilon^2.$$

Equation (3b) can be rewritten in terms of either  $T$  or  $Y$  as

$$\frac{1}{T} \frac{d^2T}{dX^2} - \ln T + \frac{\ln\lambda}{2}(w - \phi) = 0, \quad (5a)$$

$$\frac{d^2Y}{dX^2} + \frac{1}{2} \ln\lambda \left(\frac{dY}{dX}\right)^2 + w - \phi - Y = 0. \quad (5b)$$

The boundary condition is also written in terms of the scaled variables as

$$\left. \frac{d}{dX}(W_0 + \varepsilon W_1 + \mathcal{O}(\varepsilon^2)) \right|_{X=0} = \varepsilon c(W_{0s} - V_{gs}). \quad (6)$$

The value of the potential at  $x = 0$  in this paper is defined as  $w_s \equiv W_{0s}$ . Separating in orders of  $\varepsilon$  and using the boundary condition (6) to solve the resulting systems, the inner solution  $W(X) = W_0(X) + \varepsilon W_1(X) + \mathcal{O}(\varepsilon^2)$  is

$$W(X) = W_{0s} + \varepsilon c(W_{0s} - V_{gs})X + \mathcal{O}(\varepsilon^2). \quad (7)$$

This quantum inner layer solution represents the device behavior close to the interface, on the order of the reference length,  $L_D \sqrt{\ln\lambda/\lambda}$ , which has a value of 123 nm for  $\lambda = 10^6$  [7]. Equation (5b) will describe the quantum potential's coupling to the electron density in this layer.

Proceeding the quantum inner layer is the depletion outer layer, because in the subthreshold case, the device has not yet gone into inversion, thus no inversion layer is present. The equations for the outer depletion layer are

$$\frac{d^2w}{dx^2} = 1, \quad (8a)$$

$$n(x) = n_i e^{(w-\phi)\ln\lambda}. \quad (8b)$$

Expanding the depletion potential and boundary condition using  $w(x) = w_0(x) + \varepsilon w_1(x) + \mathcal{O}(\varepsilon^2)$  and grouping into orders of  $\varepsilon$ , we arrive at the following depletion layer solution:

$$w(x) = \frac{1}{2}x^2 + (a_0 + \varepsilon a_1)x + (b_0 + \varepsilon b_1) + \mathcal{O}(\varepsilon^2). \quad (9)$$

The coefficients  $(a, b) = (a_0, b_0) + \varepsilon(a_1, b_1) + \mathcal{O}(\varepsilon^2)$  are determined by matching the depletion potential on the left with the quantum layer, and on the right with a transition layer that is used to blend the solution with the bulk. To match the depletion layer with the quantum layer, an intermediate variable is introduced:

$$x_\eta = \frac{x}{\eta(\varepsilon)}, \quad \text{where} \quad \varepsilon \ll \eta(\varepsilon) \ll 1.$$

This gives  $a_0 = c(W_{0s} - v_{gs})$ ,  $b_0 = W_{0s}$ ,  $b_1 = 0$ . No information on the coefficient  $a_1$  can be extracted by the matching with the quantum layer, so this information comes by matching the depletion layer with the bulk solution,  $w_b(x) = -1 + \mathcal{O}(1/\lambda^2 \ln\lambda)$ . The matching of the depletion layer with the bulk is done in [6] by introducing a transition layer about some unknown depth  $x_d$  (referred to as the depletion width) where the proper scalings are

$$x_t = (x - x_d)(\ln\lambda)^{1/2}, \quad w = w_t(x_t) = -1 + \frac{h_0(x_t)}{\ln(\lambda)}.$$

In terms of these new scaled variables, the transition layer equation for  $h_0$  is

$$\frac{d^2h_0}{dx_t^2} = 1 - e^{-h_0},$$

where  $h_0(\infty) = 0$  is needed to match to the bulk. It is not possible to explicitly integrate this equation, however a first integral provides the implicit expression

$$-\sqrt{2}x_t = \int_1^{h_0} (e^{-y} + y - 1)^{-1/2} dy.$$

Analogous to the matching of the depletion layer with the quantum layer, we define an intermediate variable

$$x_\eta = \frac{x - x_d}{\eta(\lambda)} \quad \text{where} \quad \frac{1}{(\ln\lambda)^{1/2}} \ll \eta(\lambda) \ll 1.$$

Expanding the implicit transition layer solution as  $x_t \rightarrow \infty$  or alternatively as  $h_0 \rightarrow \infty$  provides

$$w_t(x_\eta) \sim \frac{1}{2}\eta^2 x_\eta^2 - \frac{k\eta x_\eta}{\sqrt{2\ln\lambda}} + \frac{1}{\ln\lambda} \left( \frac{k^2}{4} + 1 \right) - 1,$$

where

$$k = \int_1^\infty [(y-1)^{-1/2} - (e^{-y} + y - 1)^{-1/2}] dy \approx 0.81785.$$

See [6] for more details describing this numerical result. Expanding the depletion solution (9) using  $w(x_\eta) = w_0(x_\eta) + \varepsilon w_1(x_\eta) + \mathcal{O}(\varepsilon^2)$  in terms of the intermediate variable gives

$$w(x_\eta) = \frac{1}{2}(\eta x_\eta + x_d)^2 + c(W_{0s} - V_{gs})(\eta x_\eta + x_d) + \varepsilon a_1(\eta x_\eta + x_d) + W_{0s} + \mathcal{O}(\varepsilon^2).$$

Comparing the depletion and transition solutions to  $\mathcal{O}(1)$  and  $\mathcal{O}(\eta)$  gives the following equations

$$\begin{aligned} \mathcal{O}(1) : \quad & \frac{1}{2}x_d^2 + (c(W_{0s} - V_{gs}) + \varepsilon a_1) x_d \\ & - \frac{1}{\ln\lambda} \left( \frac{k^2}{4} + 1 \right) + W_{0s} + 1 = 0 \\ \mathcal{O}(\eta) : \quad & x_d + c(W_{0s} - V_{gs}) + \varepsilon a_1 + \frac{k}{\sqrt{2\ln\lambda}} = 0 \end{aligned}$$

Solving this system of equations for  $a_1$  and  $x_d$  gives

$$\begin{aligned} a_1 &= -\frac{1}{\varepsilon} \left[ \sqrt{2} \left( 1 + W_{0s} - \frac{1}{\ln\lambda} \right)^{1/2} + c(W_{0s} - V_{gs}) \right] \\ x_d &= \sqrt{2} \left( 1 + W_{0s} - \frac{1}{\ln\lambda} \right)^{1/2} - \frac{k}{\sqrt{2\ln\lambda}}. \end{aligned}$$

Thus, we are now able to write the full depletion layer solution  $w(x) = w_0(x) + \varepsilon w_1(x) + \mathcal{O}(\varepsilon^2)$  as

$$w(x) = \frac{1}{2}x^2 - \sqrt{2} \left( 1 + W_{0s} - \frac{1}{\ln\lambda} \right)^{1/2} x + W_{0s} + \mathcal{O}(\varepsilon^2). \quad (11)$$

This expression for the depletion layer potential agrees with the results obtained in the weak inversion-depletion analysis done in [6]. From this expression we notice that the expansion breaks down near flatband where  $w_s = -1 + \mathcal{O}(1/\ln\lambda)$  [6]. At this point, it is possible to use the boundary condition (2) for the depletion potential (11) to derive an expression for surface potential  $W_{0s}$  in terms of applied gate voltage  $V_{gs}$ . The boundary condition states that

$$\left. \frac{dw}{dx} \right|_{x=0} = c(W_{0s} - V_{gs}),$$

thus,

$$-\sqrt{2} \left( 1 + W_{0s} - \frac{1}{\ln\lambda} \right)^{1/2} = c(W_{0s} - V_{gs}).$$

Solving the above expression for  $W_{0s}(V_{gs})$  gives

$$W_{0s}(V_{gs}) = V_{gs} + \frac{1}{c^2} - \frac{\sqrt{2}}{c} \left( \frac{1}{2c^2} + 1 + V_{gs} - \frac{1}{\ln\lambda} \right)^{1/2}, \quad (12)$$

which gives an explicit value for the surface potential given any gate voltage. Analogously, solving the classical equation in the depletion region gives

$$w_s(V_{gs}) = \frac{1}{c^2} + V_{gs} - \frac{\sqrt{2}}{c} \left( \frac{1}{2c^2} + 1 + V_{gs} \right)^{1/2}. \quad (13)$$

The equations (5) relating the quantum layer potential and electron density is independent of the solution regime being examined, and consequently the solution is the same as in [7] where the strong inversion case is examined. The solution is obtained by substituting the expansion  $T = T_0 + \varepsilon T_1 + \mathcal{O}(\varepsilon^2)$  into (5a) and taking  $\mathcal{O}(1)$  terms, giving

$$\frac{d^2 T_0}{dX^2} - T_0 \ln(T_0) + \frac{\ln\lambda}{2} (W_0 - \phi) T_0 = 0,$$

where from (4) we can write

$$\begin{aligned} T_0 &= \exp(Y_0 \ln\lambda/2), \\ \tau_{0s} &\equiv T_0(\infty) = \exp((W_{0s} - \phi) \ln\lambda/2). \end{aligned}$$

Using these expressions with the quantum inner solution  $W_0(X) = W_{0s}$  and boundary condition, this  $\mathcal{O}(1)$  expression can be written as

$$\frac{d^2 S_0}{dX^2} = S_0 \ln(S_0) \quad \text{where} \quad S_0 = \frac{T_0}{\tau_{0s}}.$$

The solution to this equation is available only in implicit form, but an approximation that yields similar asymptotic results is

$$S_0(X) = \tanh(X/2),$$

which has the required behavior at  $X \ll 1$  and asymptotic decay for  $X \gg 1$  [7]. From this approximation, the expression for the quantum electron density can be expressed in terms of  $Y$  as

$$\begin{aligned} Y_0(X) &= \frac{2}{\ln\lambda} \ln(\tau_{0s} \tanh(X/2)) \\ &= W_{0s} - \phi + \frac{2}{\ln\lambda} \ln(\tanh(X/2)). \end{aligned} \quad (14)$$

In the depletion layer, the electron density behaves classically, with a straightforward expression given by (8b).

To correctly represent the composite solution throughout the entire region, the two separately calculated solutions are added together and the common terms are subtracted out. Following [7],

$$Y = \frac{1}{\ln\lambda} \ln \left( \frac{n}{n_i} \right) = w_0 + \varepsilon w_1 + Y_0 - W_{0s} + \dots$$

Thus, using this expression and solving for the electron density  $n(x)$ , the result is given by

$$n(x) = n_i \exp[(w(x) + Y_0(x) - W_{0s}) \ln \lambda], \quad (15)$$

where  $w(x)$  and  $Y_0(x)$  are given respectively by (11) and (14), and  $W_{0s}$  is the common term subtracted out.

## 4 First Integral

An interesting calculation can be done in which the governing equations in the quantum case (1) can be integrated once to give an exact expression for  $w_s(V_{gs})$ . This is done by first making the substitution  $a = \sqrt{n}$  to simplify the equations, which gives

$$w'' = \frac{a^2 - p}{N_A} + 1, \quad (16a)$$

$$w - \phi = \frac{1}{\ln \lambda} \ln \left( \frac{a^2}{n_i} \right) - \frac{\lambda \beta^2}{(\ln \lambda)^2} \frac{a''}{a}, \quad (16b)$$

where  $p = n_i \exp(-w \ln \lambda)$ . Multiplying (16a) by  $w'$  gives

$$a^2 w' = N_A (w' w'' - w') + n_i e^{-w \ln \lambda} w', \quad (17)$$

and multiplying (16b) by  $aa'$  gives

$$aa'w - \left[ \frac{a^2 \phi}{2} \right]' = \frac{1}{2 \ln \lambda} \left[ a^2 \left( 2 \ln \left( \frac{a}{\sqrt{n_i}} \right) - 1 \right) \right]' - \frac{\lambda \beta^2}{(\ln \lambda)^2} \left[ \frac{(a')^2}{2} \right]'. \quad (18)$$

Finally, we use the identity  $(a^2 w)'' = 2aa'w' + a^2 w''$  to combine (17) and (18) into a single equation in which every term can be integrated once. After integrating, we obtain

$$\frac{1}{2} \left[ a^2 w - N_A \left( \frac{1}{2} (w')^2 - w \right) + \frac{n_i}{\ln \lambda} e^{-w \ln \lambda} \right] - \frac{a^2 \phi}{2} = \frac{a^2}{2 \ln \lambda} \left( 2 \ln \left( \frac{a}{\sqrt{n_i}} \right) - 1 \right) - \frac{\lambda \beta^2}{(\ln \lambda)^2} \frac{(a')^2}{2} + \frac{K}{2}, \quad (19)$$

where  $K$  is an integration constant that is determined using the limiting values of  $w$  and  $a$  as  $x \rightarrow \infty$ . The constant works out to be

$$\frac{K}{N_A} = w_\infty + \frac{1}{\ln \lambda} \left[ \frac{2e^{-w_\infty \ln \lambda}}{\lambda} - 1 \right].$$

Now we let  $x = 0$  and use the boundary conditions  $a(0) = 0$ ,  $w(0) = w_s$ ,  $w'(0) = c(w_s - V_{gs})$  to get

$$c(w_s - V_{gs}) = -\sqrt{2} \left( w_s + \frac{e^{-w_s \ln \lambda}}{\lambda \ln \lambda} + \frac{\lambda \alpha^2 \beta^2}{N_A (\ln \lambda)^2} - \frac{K}{N_A} \right)^{1/2},$$

where  $\alpha \equiv a'(0)$ . One method of computing  $\alpha$  without requiring the complete analytic solution to the ODE's

(1a) and (1b) is to use an asymptotic expansion in  $x$  to determine  $w$  and  $a$  in a "quantum boundary layer". In [7] matched asymptotics were used to find a uniform asymptotic solution for  $w$  and  $a$  in the case of inversion,  $w_s \geq 1$ . Since we only need the value of  $\alpha$ , only the solution in this quantum boundary layer is necessary. Even though their results were for the strong inversion case, by using the first term of the asymptotic solution in this quantum layer we found that

$$\alpha = a'(0) \approx \frac{1}{\varepsilon} \sqrt{\frac{n_i \lambda \ln \lambda}{2}}.$$

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