4.1.1 $Q_s(\phi_{hs})$ relation: quantum theory

**Goal:**
- Quantum Mechanical effect on $Q_s(\phi_{hs})$
  and C-V characteristics

**Ref.** General Issues and Trend


- CMOS scaling trend requires reduction of $T_{ox}$ in order to suppress the short
  channel effect (related with the electrostatics)

- Reduction in $T_{ox}$ induces the nonideal phenomena to the device characteristics
  - Tunneling current through the thin oxide and the gate overlapped drain
    region increases the standby current ($<1\text{A/cm}^2$)
  - Effective $T_{ox}$ degradation due to QM effect in the inversion layer and the
    depletion effect in the poly silicon gate
A. Effective $T_{ox}$ degradation due to the quantum mechanical effect

- First order theory assumes that the surface potential is fixed to $2\phi_f$ which means that the inversion capacitance is infinite after the "classical $V_T$".

Then, $C_G = C_{ox}$ since $C_{inv}$ is infinite.

$$C_{inv} = \frac{\Delta Q_s}{\Delta \psi_s} = \frac{\Delta Q_n}{\Delta \psi_s}$$

However, there is certainly $\Delta \psi_s$ in order to induce $\Delta Q_n$ which means that $C_{inv}$ is finite. Then, $C_{eff}$ and $T_{eff}$ are defined as,

$$Q_n = -C_{eff}(V_G - V_T)$$

$$T_{eff} = \frac{\varepsilon}{C_{eff}}$$

. It should be noticed that the capability of storing $Q_n$ in the inversion layer is reduced due to the finite inversion layer capacitance

B. Modeling of $Q_\psi$ including the quantum mechanical effect


- In order to know the expression for $C_{eff}$, $Q_\psi(\psi_s)$ should be known. Three approaches can be taken; Classical approach with MB(Maxwell Boltzmann statistics) which is our approach in eq. (2) of §2.1, Classical approach with FD(Fermi Dirac statistics), Quantum mechanical approach.

- Quantum Mechanical Approach

The electron wave function is quantized in the potential well so that the energy states in the potential well are quantized in the depth direction. The net effect is the D(E) is not proportional to $\sqrt{E-E_c}$ in the conduction band, but constant
between the quantized energy level as shown in the figure below. This sometimes is called the "2D quantization".

\[
D_i(E) = \begin{cases} 
\frac{m^*}{\pi \hbar^2} g_s & \text{for } E \geq E_i \\
0 & \text{else}
\end{cases}
\]

where \( g_s \) is the band degeneracy.

The total DOS is
\[
D(E) = \sum_{i=0}^{\infty} D_i(E)
\]

Now areal electron density in the \( i \)th subband is
\[
N_i = \int D_i(E) f(E) dE = \int_{E_i}^{\infty} \frac{m^*}{\pi \hbar^2} \frac{1}{1 + e^{(E_i - E)/k_B T}} \ln[1 + e^{(E_i - E)/k_B T}] dE
\]

and total \( Q_n \) is
\[
Q_n = -q \sum_{i=1}^{\infty} N_i
\]

Now \( E_i \) can be only known from the Schrodinger equation as,
\[
\left[ -\frac{\hbar^2}{2m^*} \frac{d^2}{dx^2} + V_p(x) \right] \psi_i(x) = E_i \psi_i
\]

(1)
and \( V_p(x) \) is the total potential energy as the result of the Poisson equation with

\[
\rho = q(p - n + N_n) \tag{2}
\]

where \( n(x) = \sum_{r=0}^{\infty} N_r |\psi_r(x)|^2 \tag{3} \)

(1) and (2) constitute the loop to be solved numerically.

Net effect of the quantization is the reduction of the density states thereby reducing \( Q_n \) for a given \( \psi_s \) (surface potential) \( V_T \) is higher than the classical theory.

- Simplified approach based on the triangular well

Other simplified approach (approach II) is assuming "the triangular potential profile" as

\[
\psi_s(x) = \psi_s - qE_{\text{eff}} x
\]

where \( E_{\text{eff}} \) is the Effective field defined in B-1-2.

Then the solution for the Schrodinger eq. can be found as Airy function as, \( \psi_i \) with the eigen energy as

\[
E_i = \frac{3h^2}{4\sqrt{2m}} \ v_0 (i + \frac{3}{4})^{2/3} \quad \text{where} \quad i = 0, 1, 2, \ldots
\]

Then the \( n(x) \) can be found by

\[
n(x) = \sum_{r=0}^{\infty} N_r |\psi_r(x)|^2
\]

Here, \( N_i = \frac{m^* k_B T}{\pi \hbar^2} \ln \left[ 1 + e^{-\frac{E_i - E_i}{k_B T}} \right] \)

- Approach based on the Density Gradient Method

ref. S. Jin, A numerically efficient method for the hydrodynamic density-gradient model. SISPAD, pp.263-266, 2003
Fig. 1. Simulated C-V curves accounting for both QM confinement and poly-Si depletion. Simulated parameters are $d_{ox} = 3.0$ nm (2.987 nm for NEMO [19]), $N_d = 3 \times 10^{21}$ cm$^{-3}$, and $N_{poly} = 5 \times 10^{20}$ cm$^{-3}$. A classical C-V with no QM confinement or poly-Si depletion and a QM C-V which accounts for QM confinement only are also shown for illustrative purposes.

Fig. C-V curve from various models. The net effect is the degradation in CV especially for $VG > VT$.

(Fig. 1. of C. Richter’s, EDL p.35, Jan 2001)
\[ F_{DT} = F_{1-2} - F_{2-1} \]
\[ = \frac{4\pi m_e q k_B T}{\hbar^3} \int_0^{E_1} dE_2 T \left( F_2 \right) \ln \left[ \frac{1 + e^{(E_{f1} - E_{c1} - E_2)/k_B T}}{1 + e^{(E_{f2} - E_{c2} - E_2)/k_B T}} \right] \]

TC is the transmission coefficient representing the probability coefficient of the tunneling. There are several models to represent TC as function of Vox.

The transmission probability is traditionally modeled as

\[ T = e^{-2 \left( \frac{2 m e q}{\hbar^2} \right) T_{\alpha}} \]

- Simple formula
  From WKB approximation and assuming the parabolic energy band of SiO2,
  \[ T = \exp[-B0 * f(zg)] \]
  \[ zg = [1-(1-zg)]^{**1.5} / zg \]
  where \( zg = \text{Vox}/\phi \) \( b \)

- Gundlach’s formula

- Lo’s approach
  For modeling the tunneling characteristics of electrons exhibiting the 2D nature, the transmission probability applicable to an incident Fermi gas of free electrons is no longer a meaningful concept and the well known WKB approximation and the integration of the Airy functions is no valid.

Fig. from the reference indicate the modeling results from the 1st order principle (so called the transverse resonant method).

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