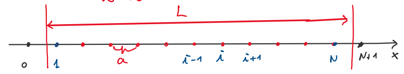
HARD WALL BOUNDARY CONDITIONS

Friday, 16 November 2018 09:00

1D domain which we discretize



In i-th point, the Schrödinger is discretized as:

$$t_0 = -\frac{\hbar^2}{2m^* a^2}$$

$$t_0 \varphi_{i-1} + (E_{ci} - 2t_0)\varphi_i + t_0 \varphi_{i+1} = E\varphi_i$$

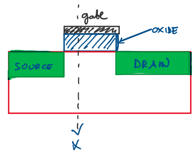
$$[H][\varphi] = E[\varphi]$$

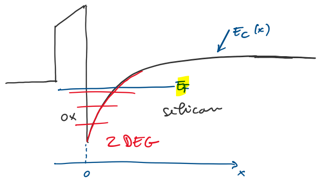
$$H = \begin{bmatrix} E_{c1}-2t_0 & t_0 & & \\ t_0 & E_{c2}-t_0 & \ddots & \\ & \ddots & \ddots & t_0 \\ & & t_0 & E_{cN}-2t_0 \end{bmatrix}$$

$$\boxed{\varphi_0 = 0 \wedge \varphi_{N+1} = 0}$$

$\downarrow$

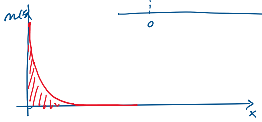
this is like considering $E_{c_0} \longrightarrow +\infty \wedge E_{c\,N+1} \longrightarrow +\infty$





Semiclassical expression for electron density

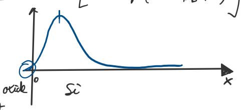
$$n(x) = N_c\, e^{-\frac{E_c(x) - E_F}{K_B T}}$$



In the case of quantum confinement:

$$n_{2DEG} = \sum_i |\varphi_i|^2 \frac{\sqrt{m_y m_t}}{\pi \hbar^2} K_B T \ln\left[1 + \exp\left(-\frac{\varepsilon_i - E_F}{K_B T}\right)\right]$$

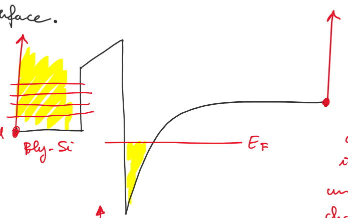
φ_i is an Airy function



φ_i penetrates the SiO_2, and the maximum is not at the interface.

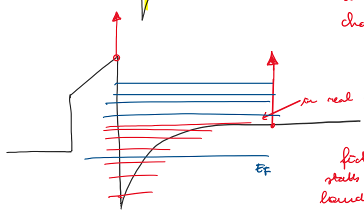
Case 1

I put the boundaries as indicated



If this is the domain I am solving, then I am introducing an artifact, i.e., quantum confinement in the gate, so I am underestimating the charge in the gate.

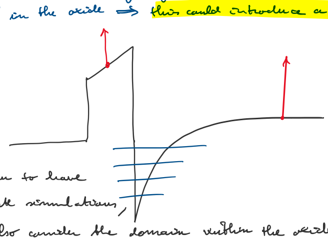
Case 2



in real case from this energy, I would have continuous states, but, here, I fictitiously include discrete states, due to the hard wall boundary conditions.

This case completely neglects the penetration of the φ in the oxide $\Longrightarrow$ this could introduce a huge error

Case 3



In order to have accurate simulations, one also consider the domain within the oxide

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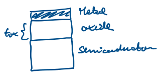
This is an MOS structure,

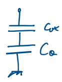


$$C = \varepsilon \cdot \frac{A}{t}$$

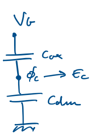
In the semi-classical case $C = \varepsilon \frac{A}{t_{ox}}$, because the charge is squeezed at the interface.

In Quantum confinement case, the centroid of charge is not at x=0 but it is right shifted

$$t_a = \frac{\int x\, n(x)\, dx}{\int x\, dx} \qquad C \triangleq \varepsilon \cdot \frac{A}{t_{ox} + t_a}$$



QM is also also leading to an increase of the threshold voltage of the MOS, due to fewer available states as compared to the semiclassical case

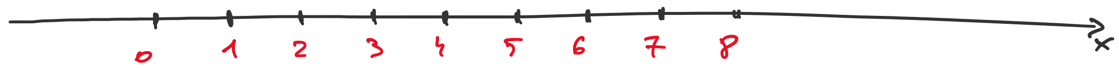


$$\phi_c = \frac{C_{ox}}{C_{ox} + C_{dm}} V_G$$

NEUMANN BOUNDARY CONDITIONS

Friday, 16 November 2018 10:14

$$\left.\frac{\delta \varphi}{\delta x}\right|_{x=0} = C \Rightarrow \frac{\varphi_1 - \varphi_0}{a} = C \Rightarrow \varphi_1 - \varphi_0 = C \cdot a = C'$$



$x=0$ $\quad \varphi_1 - \varphi_0 = C'$

$x=1$ $\quad +t_0 \varphi_0 + (E_{c1} - 2t_0)\varphi_1 + t_0 \varphi_2 = E\varphi_1$

$x=2$ $\quad t_0 \varphi_1 + (E_{c2} - 2t_0)\varphi_2 + t_0 \varphi_3 = E\varphi_2$

$\vdots$

$$\begin{bmatrix} -1 & 1 & & & \\ t_0 & E_{c1}-2t_0 & t_0 & & \\ & t_0 & E_{c2}-2t_0 & t_0 & \\ & & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} \varphi_0 \\ \varphi_1 \\ \varphi_2 \\ \vdots \\ \varphi_{N-1} \end{bmatrix} = E \begin{bmatrix} \frac{C'}{E} \\ \varphi_1 \\ \vdots \\ \varphi_{N-1} \end{bmatrix}$$