

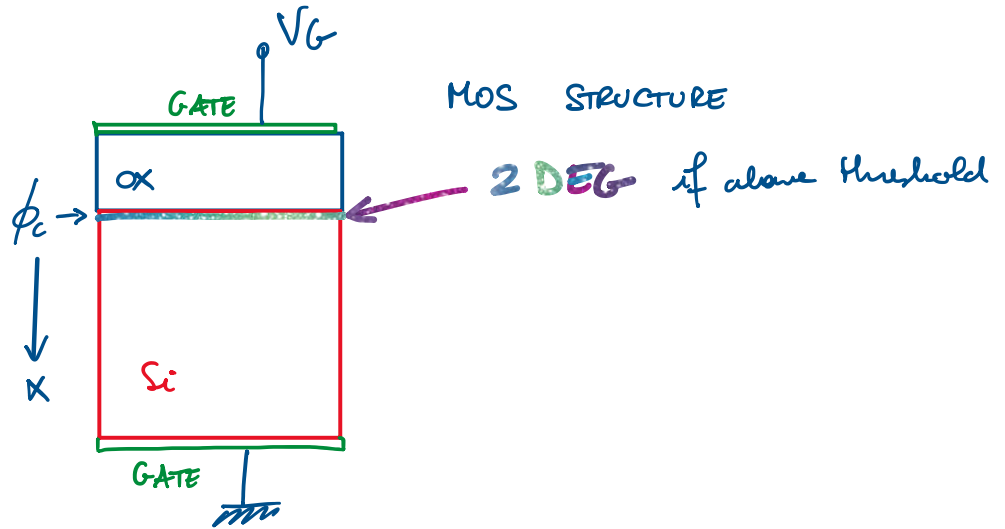
# QUANTUM CAPACITANCE

Friday, 23 November 2018 09:00

$$Q = C \cdot V$$

$$C = \frac{\delta Q}{\delta V}$$

$$C_Q = \frac{\delta Q_{2DEG}}{\delta \phi_c}$$



$$n = \sum_i^N |C_i(k)|^2 \frac{\sqrt{m_y m_z}}{\pi \hbar^2} k_B T \ln \left[ 1 + \exp \left( - \frac{E_i - E_F}{k_B T} \right) \right]$$

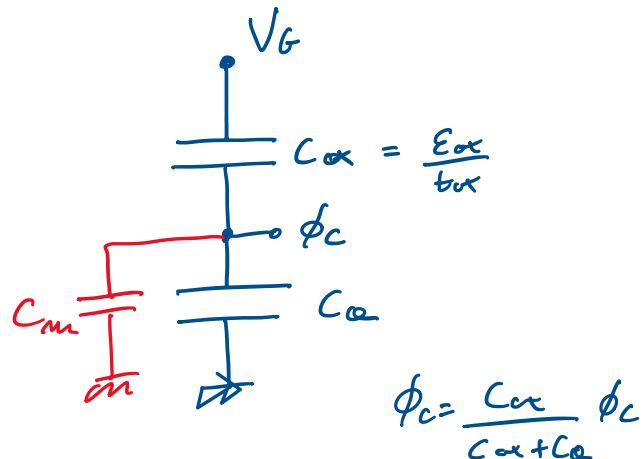
$$\int n dx \Rightarrow n_{2DEG} = \sum_i^N \frac{\sqrt{m_y m_z}}{\pi \hbar^2} k_B T \ln \left[ 1 + \exp \left( - \frac{E_i - E_F}{k_B T} \right) \right]$$

$$C_Q = \frac{\delta}{\delta \phi_c} \int q \frac{\sqrt{m_y m_z}}{\pi \hbar^2} k_B T \ln \left[ 1 + \exp \left( - \frac{E_i - E_F}{k_B T} \right) \right]$$

$E_i \approx -q \phi_c + \text{Const}$

$$C_Q = \frac{q^2 \frac{\sqrt{m_y m_z}}{\pi \hbar^2} k_B T \exp \left( - \frac{E_i - E_F}{k_B T} \right)}{1 + \exp \left( - \frac{E_i - E_F}{k_B T} \right)} \approx 1$$

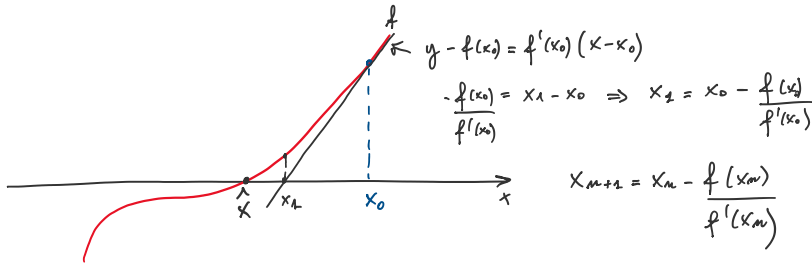
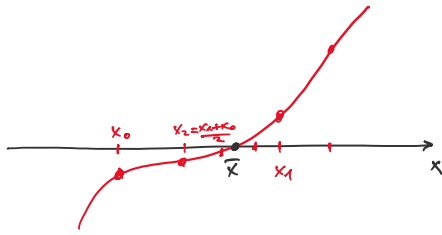
$$C_Q = \frac{\sqrt{m_y m_z}}{\pi \hbar^2} q^2 = \text{DOS}_{2D} \cdot q^2$$



# Newton Method

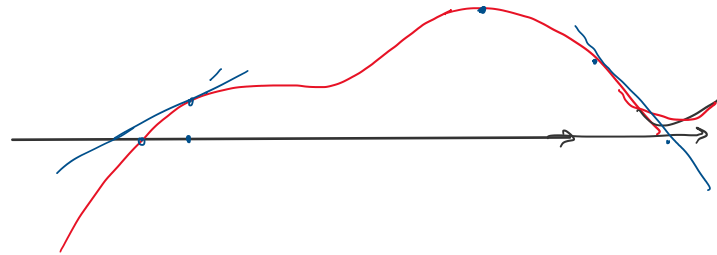
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$$f(x) = 0$$



$$\begin{cases} f_1(\phi_1, \phi_2, \dots, \phi_{np}) = 0 \\ f_2(\phi_1, \phi_2, \dots, \phi_{np}) = 0 \\ \vdots \\ f_{np}(\phi_1, \phi_2, \dots, \phi_{np}) = 0 \end{cases} \quad \vec{f}(\vec{\phi}) : \mathbb{R}^n \rightarrow \mathbb{R}^m$$

$$f_i \rightarrow J(\phi) = \begin{pmatrix} \frac{\partial f_1}{\partial \phi_1} & \frac{\partial f_1}{\partial \phi_2} & \dots & \frac{\partial f_1}{\partial \phi_{np}} \\ \frac{\partial f_2}{\partial \phi_1} & \frac{\partial f_2}{\partial \phi_2} & \dots & \frac{\partial f_2}{\partial \phi_{np}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_{np}}{\partial \phi_1} & \dots & \dots & \frac{\partial f_{np}}{\partial \phi_{np}} \end{pmatrix}$$



$$\vec{f}(\vec{\phi}) = 0 \quad \vec{\phi}_k \quad \vec{f}(\vec{\phi}_k) = \vec{r}_k \leftarrow \text{residual}$$

$\uparrow$  exact solution       $\uparrow$  trial solution

$$\vec{\phi} = \vec{\phi}_k + d\vec{\phi}_k$$

$$\vec{f}(\vec{\phi}) = \vec{f}(\vec{\phi}_k + d\vec{\phi}_k) = 0 \quad \|d\vec{\phi}_k\| \ll \|\vec{\phi}_k\|$$

$$\vec{f}(\vec{\phi}_k + d\vec{\phi}_k) = \underbrace{\vec{f}(\vec{\phi}_k)}_{\vec{r}_k} + J(\vec{\phi}_k) \cdot d\vec{\phi}_k = 0$$

$$J(\vec{\phi}_k) \cdot d\vec{\phi}_k = -\vec{r}_k \Rightarrow \underline{d\vec{\phi}_k} = -J^{-1}(\vec{\phi}_k) \cdot \vec{r}_k$$

$$\vec{\phi}_{k+1} = \vec{\phi}_k + d\vec{\phi}_k$$

NUMERICAL RECIPES  $\left\{ \begin{array}{l} \text{IN FORTRAN ??} \\ \text{IN C} \end{array} \right.$