1D confinement

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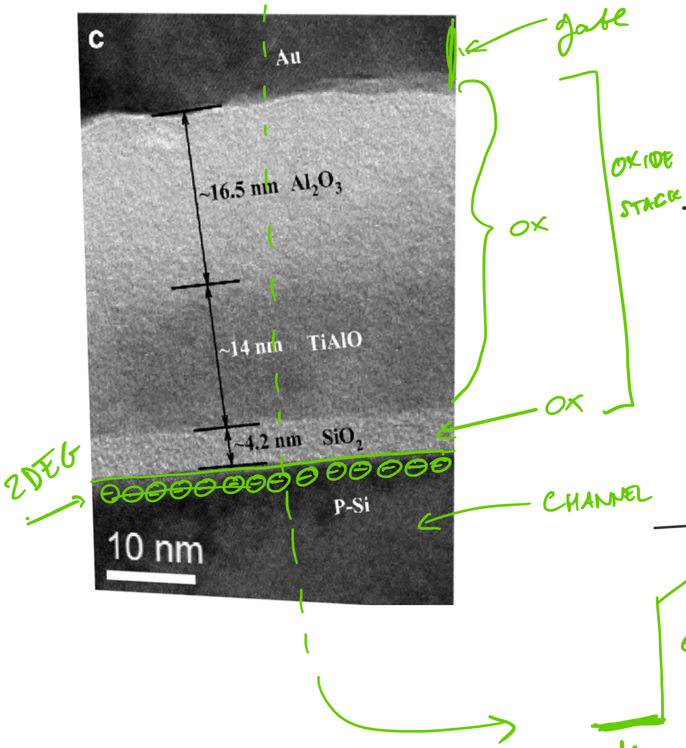
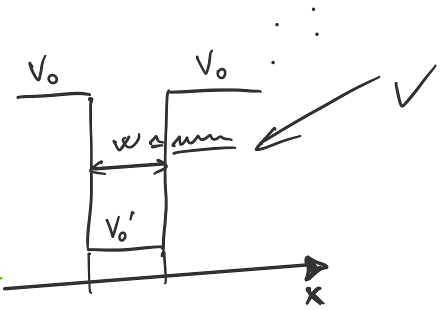
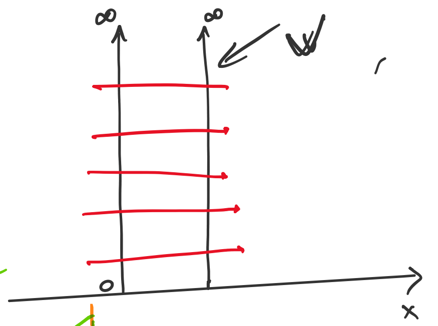
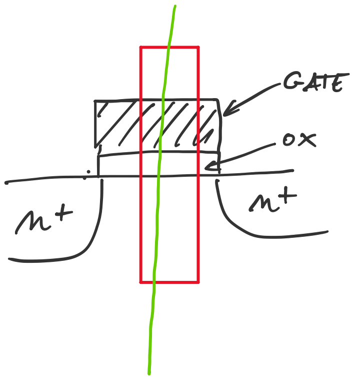
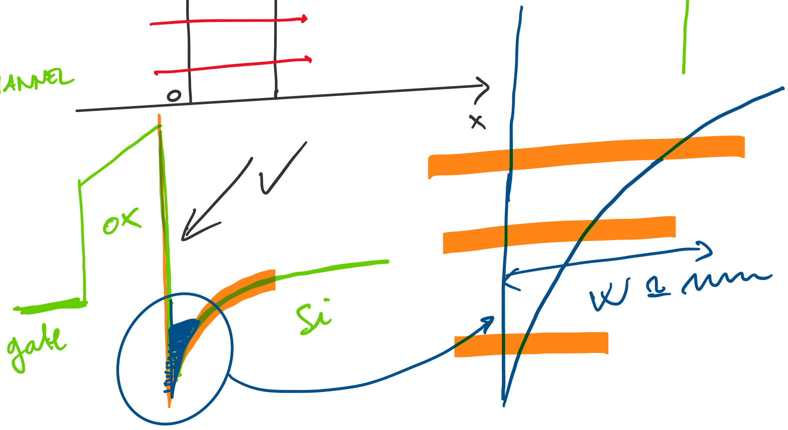
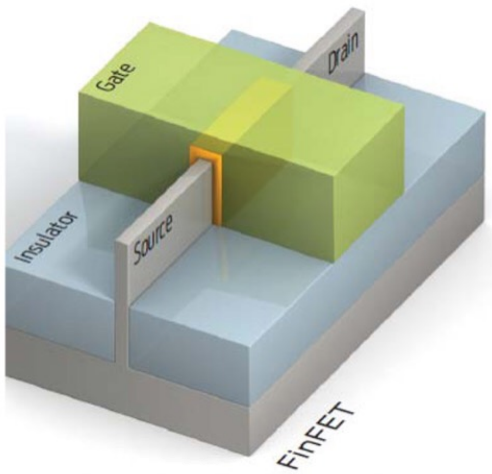




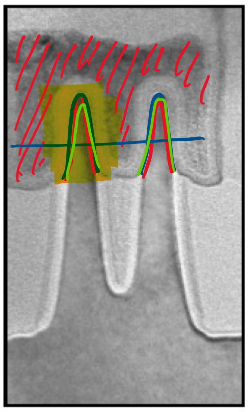


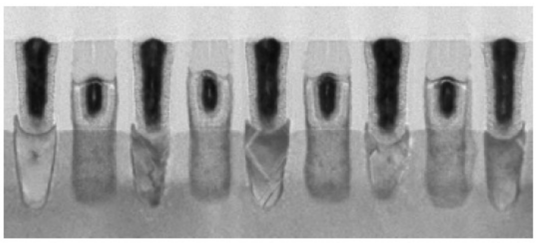


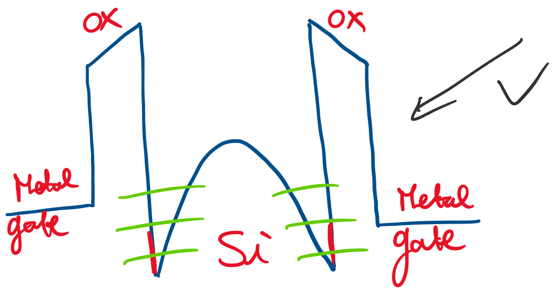




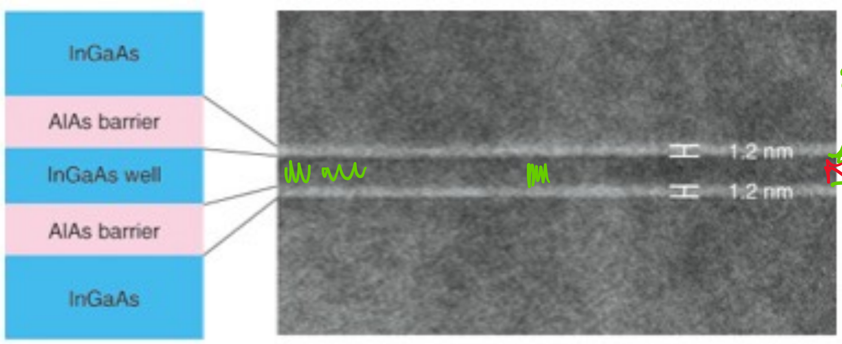
14nm-class FinFET transistor



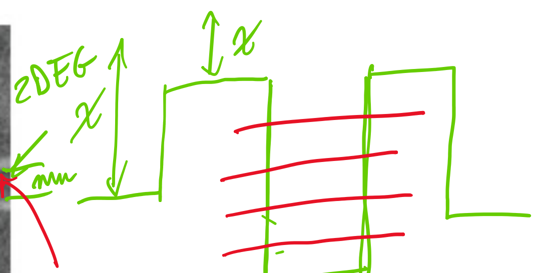




III - V



(a) (b)



2D confinement

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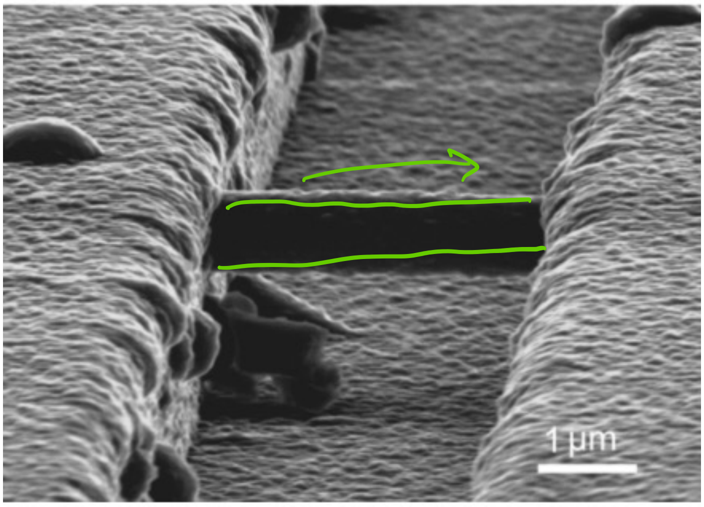
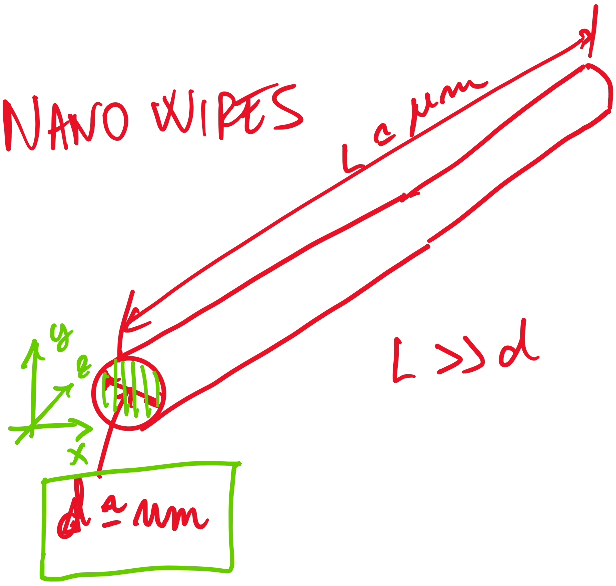
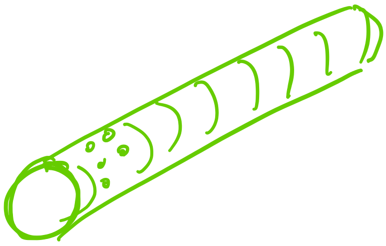


CARBON NANOTUBES

NANO WIRES



$L >> d$



3D Confinement

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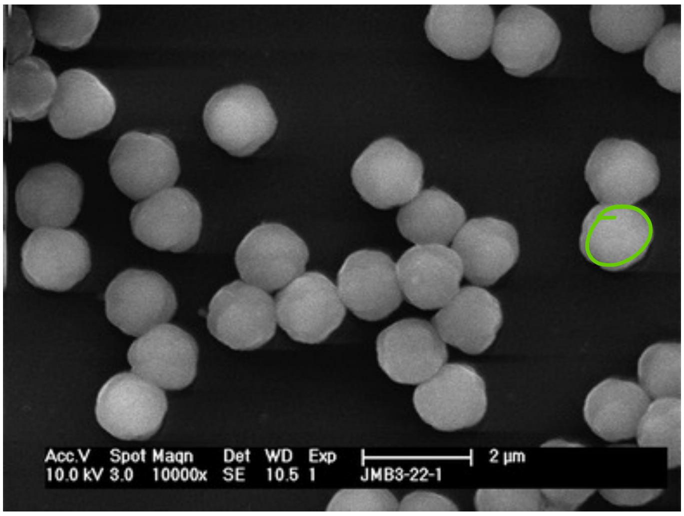
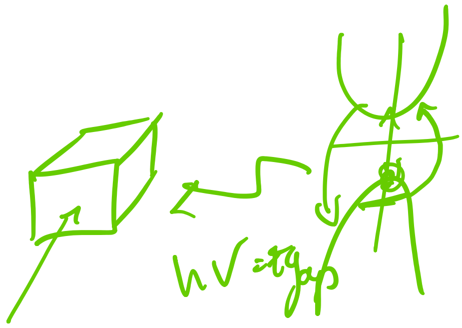
QUANTUM DOT





DISCRETIZATION

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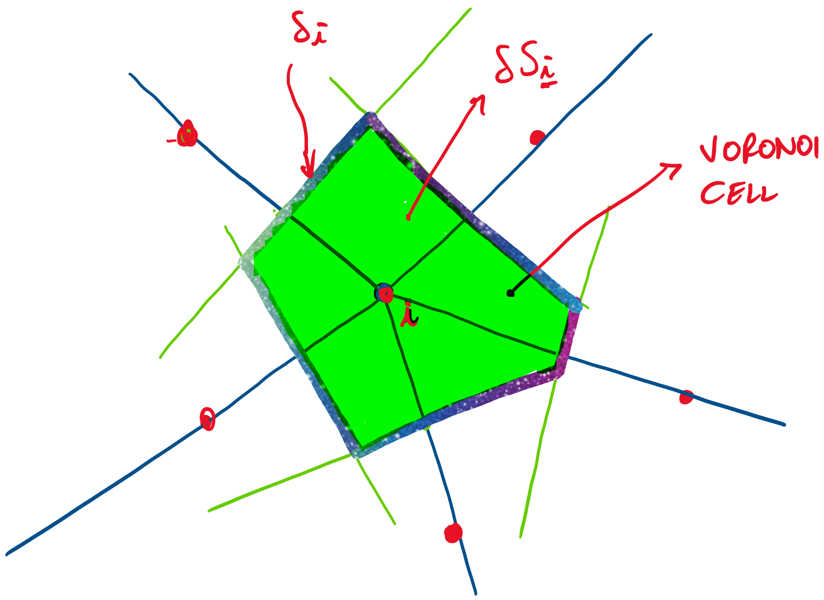
$eg(x) = 0$

<u>CAD</u> <u>ANSYS</u>

BOX INTEGRATION METHOD

$$\boxed{-\frac{\hbar^2}{2}\underline{\nabla}\cdot\left(\frac{1}{m}\underline{\nabla}\varphi\right)+V\varphi=\underline{E}\varphi}$$

2D



$$\int_{\delta S_i} -\frac{\hbar^2}{2}\underline{\nabla}\cdot\left(\frac{1}{m}\underline{\nabla}\varphi\right)dS+\int_{\delta S_i} V\varphi\, dS=\int_{\delta S_i} E\varphi\, dS$$

$$\underbrace{\int_{\delta S_i} -\frac{\hbar^2}{2}\underline{\nabla}\cdot\left(\frac{1}{m}\underline{\nabla}\varphi\right)dS}_{\text{to solve this term, we use the GAUSS-GREEN theorem}} + V_i\varphi_i\,\delta S_i = E\varphi_i\int_{\delta S_i} dS = E\varphi_i\,\delta S_i$$

I have assumed that the VORONOI cell is sufficiently small that all the quantities within the VORONOI CELL are constant

GAUSS - GREEN THEOREM

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we want to solve:

$$-\frac{\hbar^2}{2}\int_{\delta S_i} \underline{\nabla}\cdot\left(\frac{1}{m}\underline{\nabla}\varphi\right)\cdot dS$$

For GAUSS- GREEN

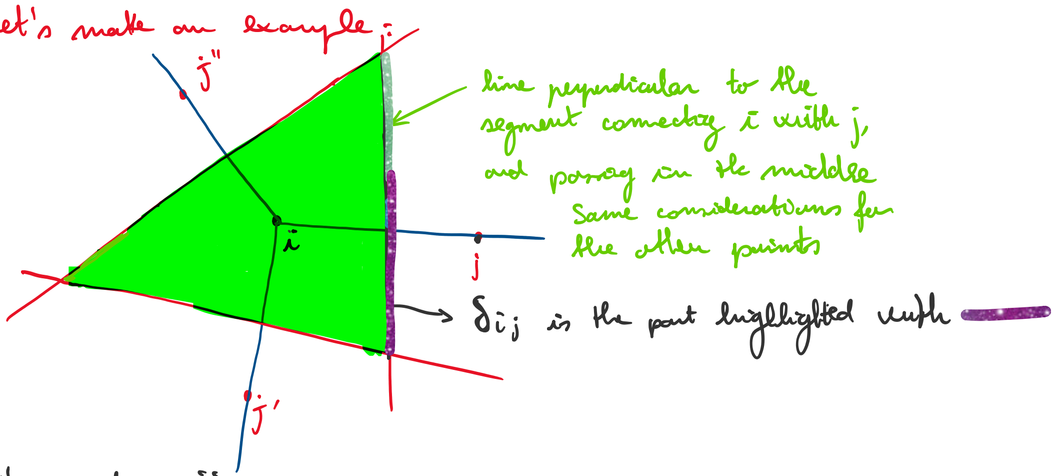
$$\int_{\delta S}\underline{\nabla}\cdot\underline{F}\,dS = \oint_{\delta l}\underline{F}\cdot d\underline{l}$$

where δS is the domain and δl is the region delimiting the domain

Applying GAUSS- GREEN, we obtain

$$\boxed{-\frac{\hbar^2}{2}\oint_{\delta l_i}\frac{1}{m}\underline{\nabla\varphi}\cdot d\underline{\hat{n}}}$$

Let's make an example:



Let's consider ij

the $\nabla\varphi$ along ij direction is discretized as follows:

$\frac{\varphi_j-\varphi_i}{d_{i,j}}$, where $d_{i,j}$ is the distance between i and j points

the flux over the line δ_{ij} can be written as:

$$\boxed{-\frac{\hbar^2}{2}\,\frac{1}{\frac{m_i+m_j}{2}}\,\frac{\varphi_j-\varphi_i}{d_{ij}}\cdot\delta_{ij}}$$

This is the term for ij, but we have other first neighbours.

So in general, for N first neighbours, the equation can be written as:

$$\boxed{-\frac{\hbar^2}{2}\sum_{j=1}^{N}\frac{1}{\frac{m_i+m_j}{2}}\cdot\frac{\varphi_j-\varphi_i}{d_{ij}}\cdot\delta_{ij}}$$