

# **EE-612:**

## **Lecture 6**

# **Quantum Mechanical Effects**

**Mark Lundstrom**  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, IN USA  
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**NCN**

[www.nanohub.org](http://www.nanohub.org)

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## outline

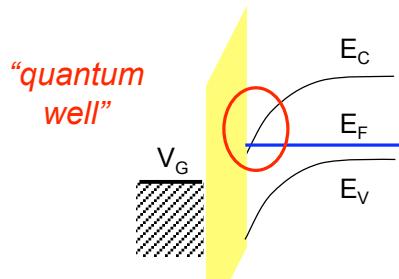
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- 1) Review
- 2) Quantum confinement fundamentals
- 3) Quantum capacitance
- 4) Schrödinger-Poisson simulation
- 5) Simulation examples

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## quantum confinement in an MOS-C



$$p = \hbar k = \hbar \frac{2\pi}{\lambda}$$

$$E = \frac{p^2}{2m^*}$$

$$\langle E \rangle = \frac{\langle p^2 \rangle}{2m^*} = \frac{3}{2} k_B T$$

$$\lambda_D = \frac{\hbar}{\sqrt{3m^* k_B T}} \approx 10 \text{ nm} \quad (\text{Si})$$

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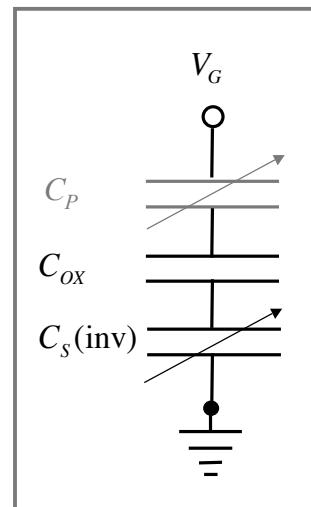
## inversion layer capacitance

$$Q_i = Q_i(V_T) + \frac{\partial Q_i}{\partial V_G} (V_G - V_T) + \dots$$

$$V_G = V_{FB} + \psi_s - \frac{Q_i}{C_{ox}} \quad (V_G \gg V_T)$$

$$\frac{\partial V_G}{\partial (-Q_i)} = \frac{\partial \psi_s}{\partial (-Q_i)} + \frac{1}{C_{ox}}$$

$$\frac{1}{C_G} = \frac{1}{C_s(\text{inv})} + \frac{1}{C_{ox}}$$



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## inversion layer capacitance

$$C_s(\text{inv}) \equiv \frac{\partial Q_i}{\partial \psi_s} \equiv \frac{\epsilon_{Si}}{t_{inv}}$$

want:  $C_s(\text{inv}) \gg C_{ox}$       so:  $C_G = \frac{C_{ox}C_s(\text{inv})}{C_{ox} + C_s(\text{inv})} \approx C_{ox}$

classically:

$$C_s(\text{inv}) = \frac{Q_i}{(2k_B T/q)} \equiv \frac{C_{ox}(V_G - V_T)}{(2k_B T/q)} \sim \frac{1\text{V}}{0.05\text{V}} \sim 10 - 20$$

quantum mechanics and Fermi-Dirac statistics reduce  $C_s(\text{inv})$ , which decreases  $C_G$  and increases  $EOT_{elec}$

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- 1) Review
- 2) **Quantum confinement fundamentals**
- 3) Quantum capacitance
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- 5) Simulation examples

## particle in a box: Schrödinger equation

$$-\frac{\hbar^2}{2m^*} \frac{d^2\psi(x)}{dx^2} + U(x)\psi = E\psi$$

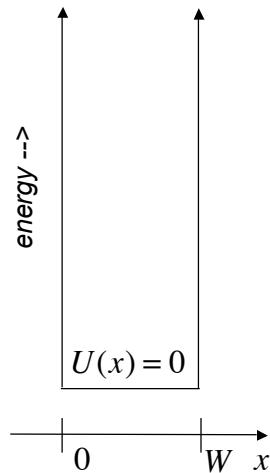
$$n(x) \approx \psi^*(x)\psi(x)$$

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m^*E}{\hbar^2}\psi = 0$$

$$\boxed{\frac{d^2\psi(x)}{dx^2} + k^2\psi = 0}$$

$$k^2 = \frac{2m^*E}{\hbar^2}$$

$$E = \frac{\hbar^2 k^2}{2m^*}$$



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## particle in a box: confined wavefunctions

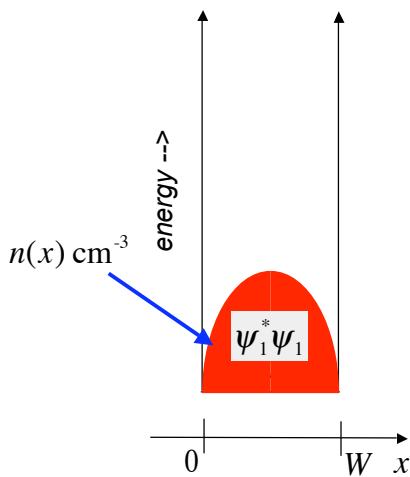
$$\frac{d^2\psi(x)}{dx^2} + k^2\psi = 0$$

$$\psi(0) = \psi(W) = 0$$

$$\psi(x) = \sin kx$$

$$kW = n\pi \quad k_n = \frac{n\pi}{W}$$

$$\psi_n(x) = \sin \frac{n\pi x}{W}$$



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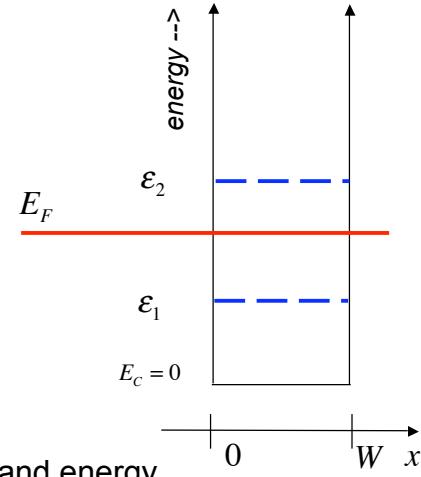
## energy levels

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi = 0$$

$$\psi(x) = \sin k_n x$$

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2m^* W^2}$$

light mass  
narrow width  $\Rightarrow$  high subband energy



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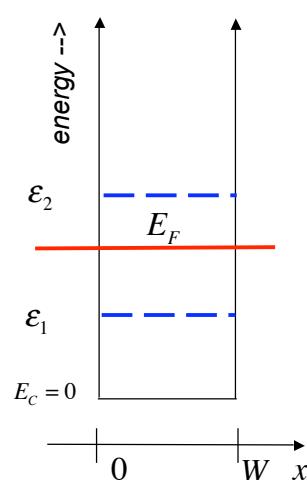
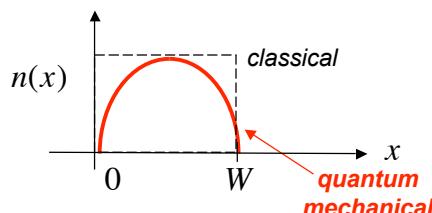
## carrier densities

classically:

$$n(x) = N_C F_{1/2} [(E_F - E_C)/k_B T] \text{ cm}^{-3}$$

quantum mechanically:

$$n(x) \sim \psi^*(x)\psi(x) \text{ cm}^{-3}$$



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## carrier densities (ii)

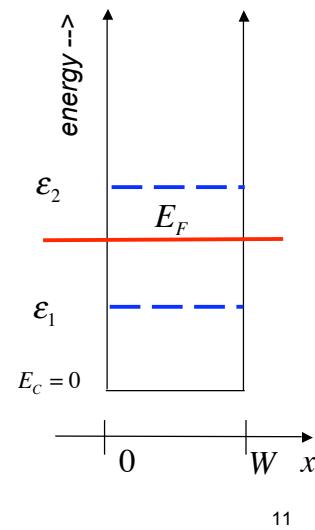
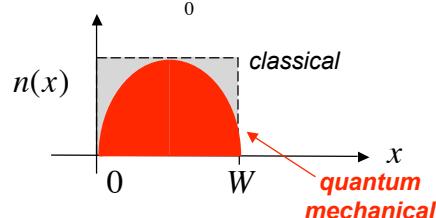
$$n_s = \int_0^W n(x) dx \text{ cm}^{-2}$$

classical:

$$n_s = N_C F_{1/2} [(E_F - E_C)/k_B T] W$$

quantum mechanical:

$$n_s \sim \int_0^W \psi^*(x) \psi(x) dx$$



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## carrier densities (iii)

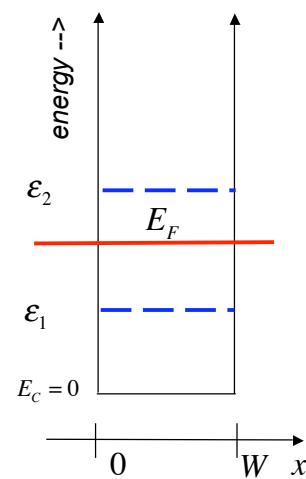
$$n_s = \int_0^W n(x) dx \text{ cm}^{-2}$$

$$n_s = \int_0^\infty g_{2D}(E) f_0(E) \text{ cm}^{-2}$$

$$g_{2D}(E) = \frac{m^*}{\pi \hbar^2}$$

$$n_s = N_C^{2D} \ln \left( 1 + e^{(E_F - \varepsilon)/k_B T} \right)$$

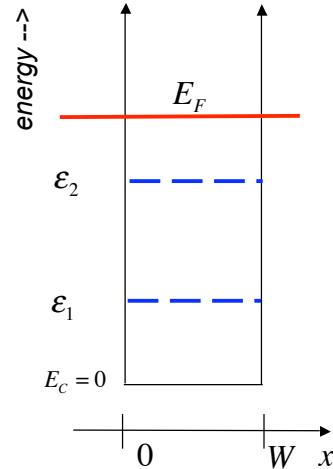
$$n_s = N_C^{2D} F_0 \left[ (E_F - \varepsilon) / k_B T \right] \text{ cm}^{-2}$$



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## carrier densities (iv)

$$n_s = \sum_{i=1}^N N_{ci}^{2D} F_0 [(E_F - \varepsilon_i) / k_B T] \text{ cm}^{-2}$$



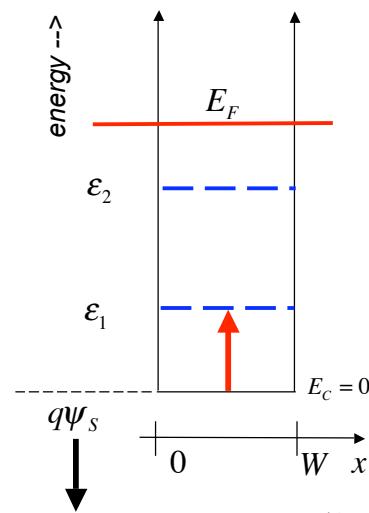
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## QM shift of V\_T

- to first order, QM simply raises  $E_C$  by  $\varepsilon_1$
- $\psi_s$  must increase by  $\Delta\psi_s^{QM}$  to achieve inversion

$$\begin{aligned} \psi_s &= 2\psi_B \\ \Rightarrow \\ \psi_s &= 2\psi_B + \Delta\psi_s^{QM} \end{aligned}$$

$$\Delta\psi_s^{QM} \simeq \varepsilon_1 / q$$



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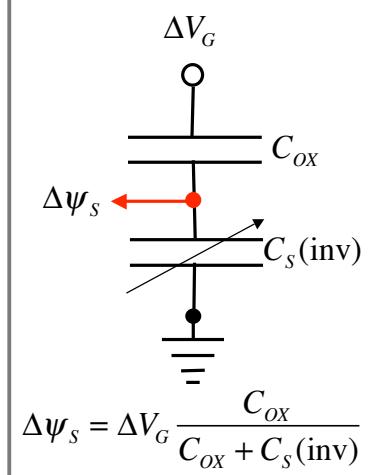
## QM shift of $V_T$ (ii)

$$\Delta\psi_s^{QM} \approx \epsilon_1 / q$$

$$\Delta\psi_s = \frac{\Delta V_G}{m} \quad m = 1 + C_s(\text{inv})/C_{ox}$$

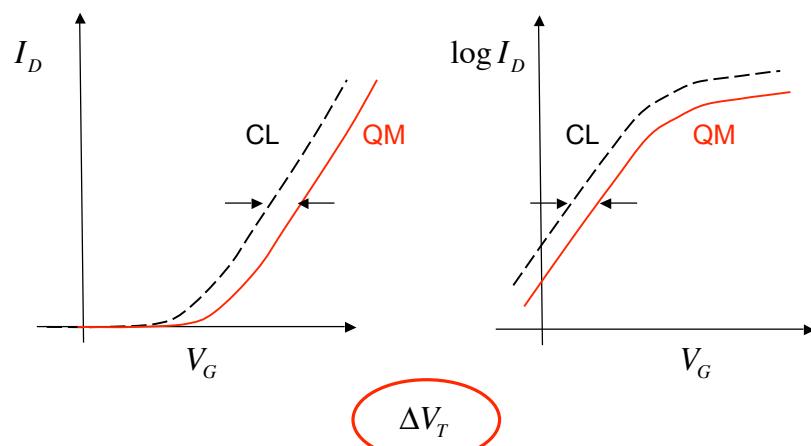
$$\Delta V_T = m \Delta\psi_s^{QM}$$

$$V_T = V_{FB} + 2\psi_B + m \Delta\psi_s^{QM} - \frac{Q_D(2\psi_B)}{C_{ox}}$$

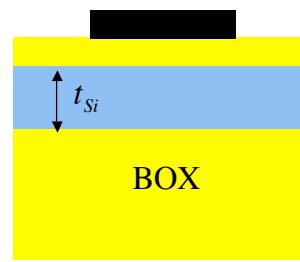
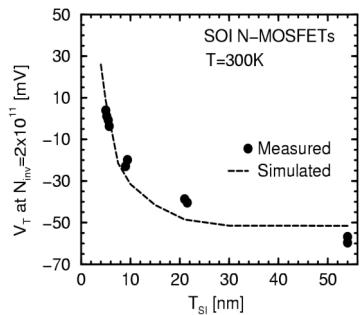


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## QM shift $V_T$ (iii)

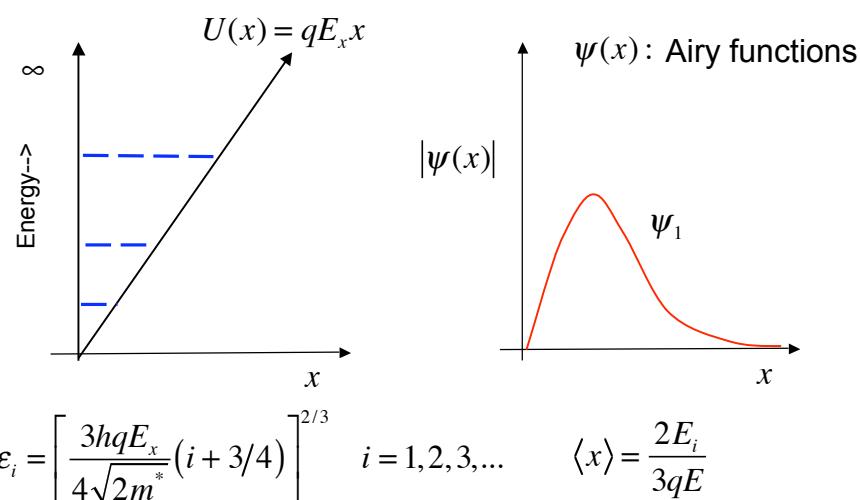


## QM shift $V_T$ (iv)

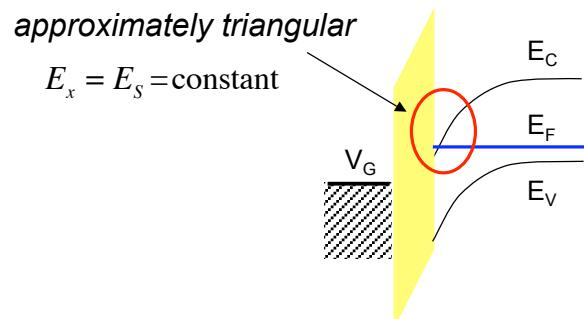


(D.Esseni et al. IEDM 2000 and TED 2001)

## triangular quantum well



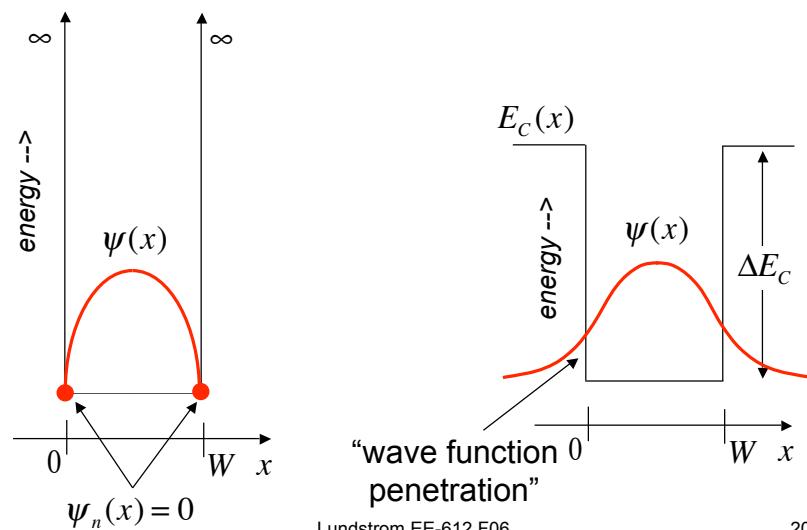
## triangular quantum well



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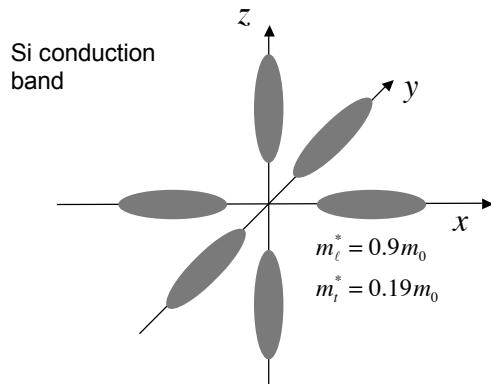
## infinite vs. finite height quantum well



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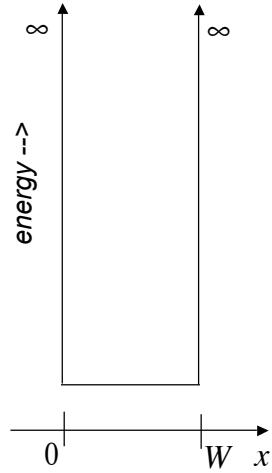
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## bandstructure effects on QM confinement



$$E_n = \frac{\hbar^2 n^2 \pi^2}{2m^*}$$

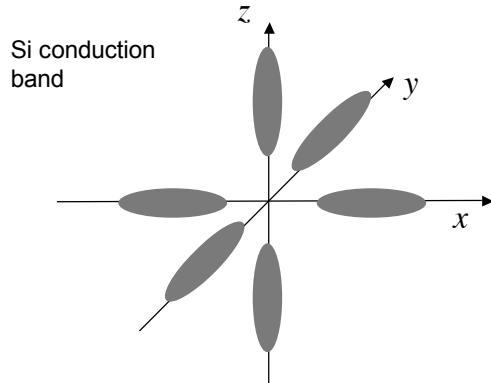
$m^* = ?$



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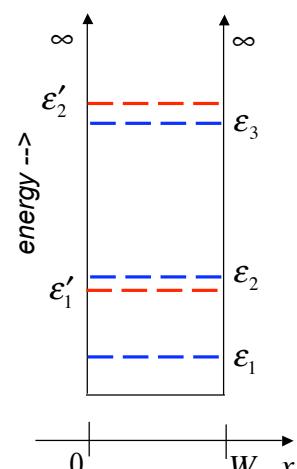
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## bandstructure effects on QM confinement



unprimed ladder:  $m^* = m_\ell^*$   $g = 2$

primed ladder:  $m^* = m_t^*$   $g = 4$



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## bandstructure effects on QM confinement

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$$n_s^i = \frac{g_i m_i^* k_B T}{\pi \hbar^2} F_0 \left[ (E_F - \epsilon_i) / k_B T \right] \text{cm}^{-2}$$

unprimed subbands:

$$m_i^* = m_\ell^* \quad g_i = 2$$

primed subbands:

$$m_i^* = m_t^* \quad g_i = 4$$

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## semiconductor capacitance

$$C_s(\text{inv}) \equiv \frac{\partial(-Q_i)}{\partial \psi_s}$$

$$Q_i = -q \int_{\epsilon_1 + E_C} g_{2D} f_0(E - E_F) dE$$

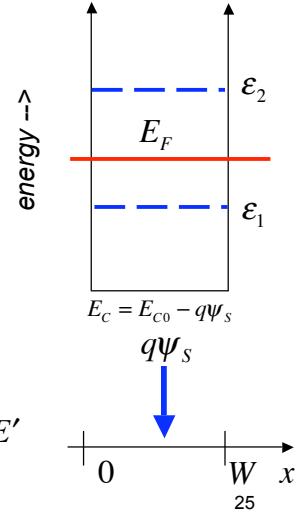
$$E' = E - \epsilon_1 - E_C$$

$$Q_i = -q \int_0 g_{2D} f_0(E' + \epsilon_1 + E_C - E_F) dE'$$

$$E_C = E_{C0} - q\psi_s$$

$$Q_i = -q \int_0 g_{2D} f_0(E' - q\psi_s + \epsilon_1 + E_{C0} - E_F) dE'$$

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## quantum capacitance

$$Q_i = -q \int_0 g_{2D} f_0(E' - q\psi_s + \epsilon_1 + E_{C0} - E_F) dE'$$

$$C_s = \frac{\partial(-Q_i)}{\partial \psi_s} = q \int_0 g_{2D} \frac{\partial f_0}{\partial \psi_s} dE' \quad [\text{now assume that } \epsilon_1 \neq f(\psi_s)]$$

$$\frac{\partial f_0}{\partial \psi_s} = -q \frac{\partial f_0}{\partial E'}$$

$$C_s = C_Q = q^2 \int_0 g_{2D} \left( -\frac{\partial f_0}{\partial E'} \right) dE'$$

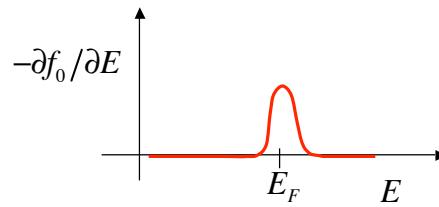
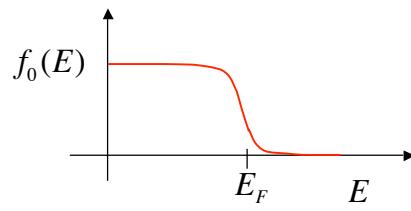
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## quantum capacitance (ii)

$$C_Q = q^2 \int_0 g_{2D} \left( -\frac{\partial f_0}{\partial E'} \right) dE'$$

$$C_Q = q^2 \langle g_{2D}(E_F) \rangle$$



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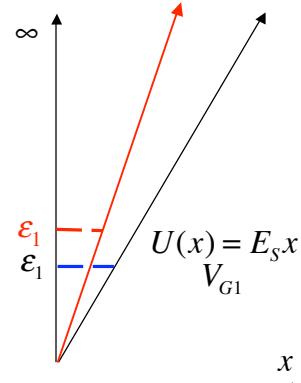
## $C_Q$ vs. $C_S$

$$Q_i = -q \int_0 g_{2D} f_0 (E' - q\psi_s + \varepsilon_1 + E_{C0} - E_F) dE'$$

$$V_{G2} > V_{G1}$$

$$\frac{\partial(-Q_i)}{\partial\psi_s} = \frac{\partial(-Q_i)}{\partial\psi_s} + \frac{\partial(-Q_i)}{\partial\varepsilon_1} \frac{\partial\varepsilon_1}{\partial\psi_s}$$

$$C_S = C_Q \left[ 1 - \frac{\partial(\varepsilon_1/q)}{\partial\psi_s} \right] < C_Q$$



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## QM effects on $C_S(\text{inv})$

assume  $C_S \approx C_Q$

$$C_Q = q^2 \frac{g_{2D}(E_F - \varepsilon_1)}{(E_F - \varepsilon_1)} = \frac{Q_i}{(E_F - \varepsilon_1)/q} \quad \text{assumes } T = 0\text{K or highly degenerate}$$

recall:

$$C_Q(\text{classical, Boltzmann}) = Q_i / (2k_B T / q)$$

$$\text{for: } Q_i = -q \times 10^{13} \quad (E_F - \varepsilon_1) \approx 4k_B T$$

$$C_Q(QM) \approx \frac{1}{2} C_Q(\text{CL, Boltzmann})$$

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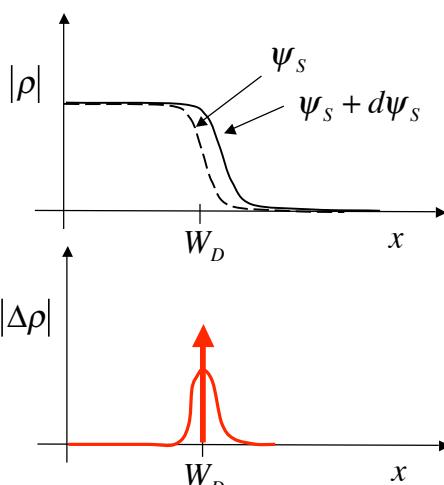
## another view of how QM affects $C_S(\text{inv})$

$$0 < \psi_S < 2\psi_B$$

$$C_S = C_D$$

$$C_D = \frac{|\Delta\rho|}{\Delta\psi_S}$$

$$C_D = \frac{\varepsilon_{Si}}{W_D}$$



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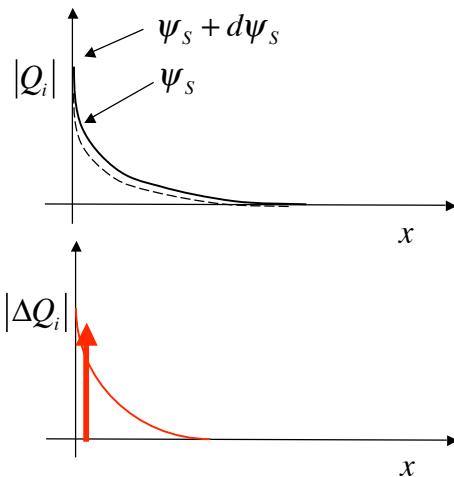
## another view: classical (ii)

$$2\psi_B < \psi_S$$

$$C_s = C_s(\text{inv})$$

$$C_s(\text{inv}) = \frac{|\Delta Q_i|}{\Delta \psi_s}$$

$$C_s(\text{inv}) = \frac{\epsilon_{Si}}{t_{\text{inv}}(CL)}$$



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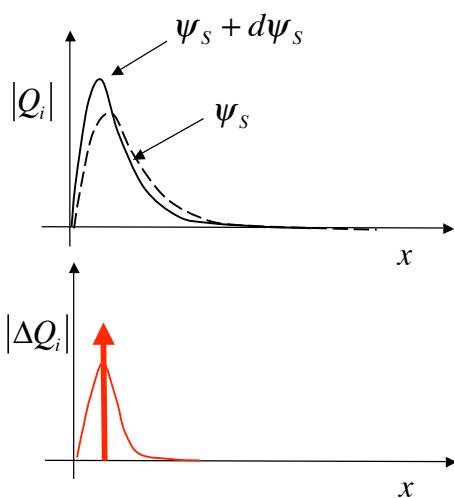
## another view: quantum mechanical

$$2\psi_B < \psi_S$$

$$C_s = C_s(\text{inv})$$

$$C_s(\text{inv}) = \frac{|\Delta Q_i|}{\Delta \psi_s}$$

$$C_s(\text{inv}) = \frac{\epsilon_{Si}}{t_{\text{inv}}(QM)}$$



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## summary

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### ***Quantum mechanics:***

- 1) increases  $V_T$
- 2) decreases  $C_S$  (inv) and, therefore,  $C_G$ (on)

$$t_{inv}(QM) > t_{inv}(CL)$$

$$EOT_{elec} = \left( \frac{\kappa_{OX}}{\kappa_{ins}} \right) t_{ins} + \left( \frac{\kappa_{OX}}{\kappa_{Si}} \right) t_{inv}$$

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## Schrödinger-Poisson simulation

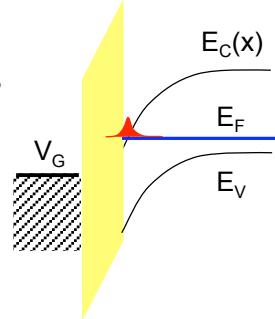
In general,  $E_C(x)$  and  $n(x)$  must be computed self-consistently by solving the Schrödinger and Poisson equations self-consistently.

(1)

$$\text{Wave Equation} \\ E_C(\mathbf{r}) \rightarrow n(\mathbf{r})$$

(2)

$$\text{"Poisson" Equation} \\ n(\mathbf{r}) \rightarrow E_C(\mathbf{r})$$



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## Schrödinger-Poisson simulation (1)

$$\left[ -\frac{\hbar^2}{2} \frac{d}{dx} \frac{1}{m_i^*} \frac{d}{dx} + E_C(x) \right] \psi_{i,j}(x) = \epsilon_{i,j} \psi_{i,j}$$

index,  $i$ , labels ladder (unprimed or primed) and index,  $j$ , is the eigenvalue

$$E_C(x) = -qV(x) + \Delta E_C$$

$$n(x) = \frac{k_B T}{\pi \hbar^2} \sum_I g_i m_{di}^* \sum_j \ln \left[ 1 - e^{(E_F - \epsilon_{i,j})/k_B T} \right] |\psi_{i,j}|^2$$

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## Schrödinger-Poisson simulation (2)

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$$\frac{d}{dx} \left[ \epsilon(x) \frac{d}{dx} \right] V(x) = \frac{q}{\epsilon_{Si}} \left[ n(x) - p(x) + N_A^- + N_D^+ \right]$$

For more information on Schrödinger-Poisson, simulation, see:

S.-H. Lo, D.A. Buchanan, and Y. Taur, *IBM J. Res. and Dev.*, **43**, p. 327, 1999.

D. Vasileska, et al., *IEEE Trans. Electron Dev.*, **44**, p. 584, 1997.

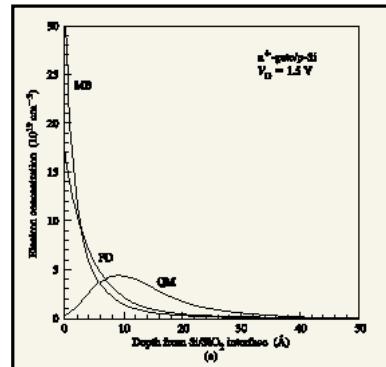
also see the simulation program, Schred, at [www.nanoHUB.org](http://www.nanoHUB.org)

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## simulation results



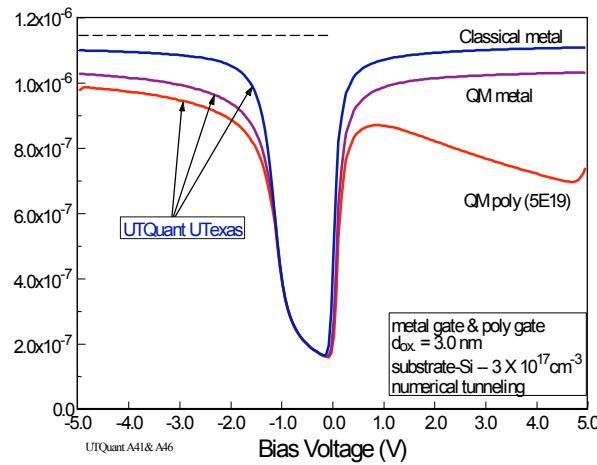
Results from S.H. Lo, et al., *IBM J. Research and Development*, **43**, no. 3, pp. 327-337, May 1999

## simulation results

Example MOS C-V Simulations  
from Curt Richter, NIST

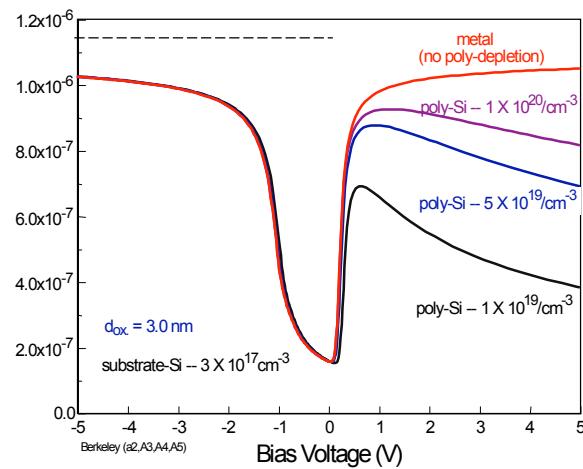
Similar capabilities are provided by Schred on  
the nanoHUB ([www.nanoHUB.org](http://www.nanoHUB.org))

## simulation results



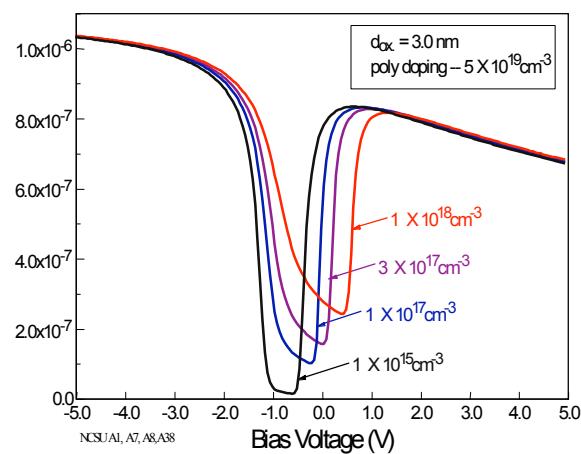
UTQUANT 2.0 User's Guide: Shih, Jallepalli, Chindalore, Hareland, Maziar, and Tasch

## simulation results



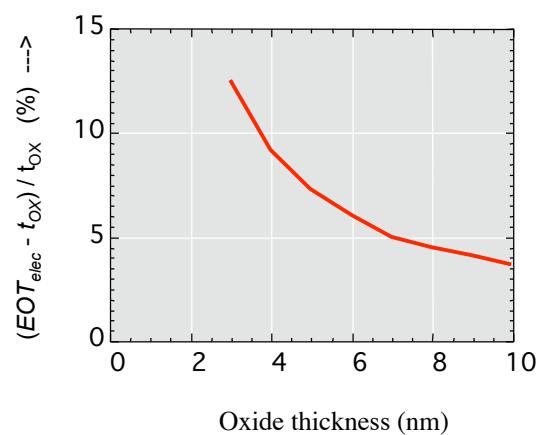
UC Berkeley Device Group  
[www-devices.eecs.berkeley.edu/~kjyang/qmcv/index.html](http://www-devices.eecs.berkeley.edu/~kjyang/qmcv/index.html) 42

## simulation results



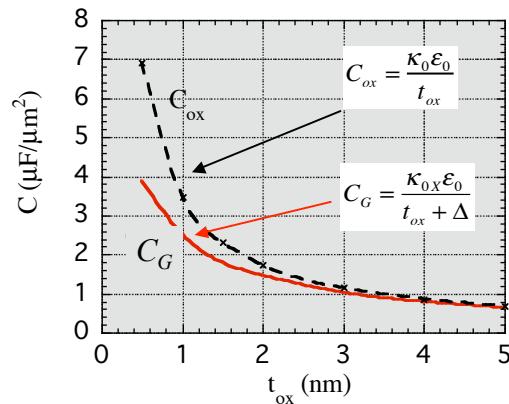
J.R. Hauser and K. Ahmed, in Characterization and Metrology for ULSI Technology, Seiler et al eds. 1998, p.235.

## effect of QM on EOT



( after Vasileska, et al., *IEEE TED*, **44**, 584, 1997)

## effect of QM on $t_{ox}$ scaling



( see Vasileska, et al., *IEEE TED*, **44**, 584, 1997)

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