Improved Compact Model of Quantum Sub-band Energy Levels for MOSFET Device Application

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Outline

- Triangular potential well approximation.
- WKB approach.
- Self-Consistent Schrödinger-Poisson (SP) numerical approach.
- Compact model with quantum effect.
- Results and comparisons.
- Conclusion.
- Exponential approximation of the potential energy.

Triangular potential well approximation

- 1-D Schrödinger equation

$$\frac{d^2\psi_j}{dx^2} + \frac{2m^*}{\hbar^2}[E_j - U]\psi_j = 0$$

- Where *m*=0.916*m_e is electron effective mass in the direction perpendicular to the transistor channel surface, $U(x) = -qF_s x$ and F_s the surface field.

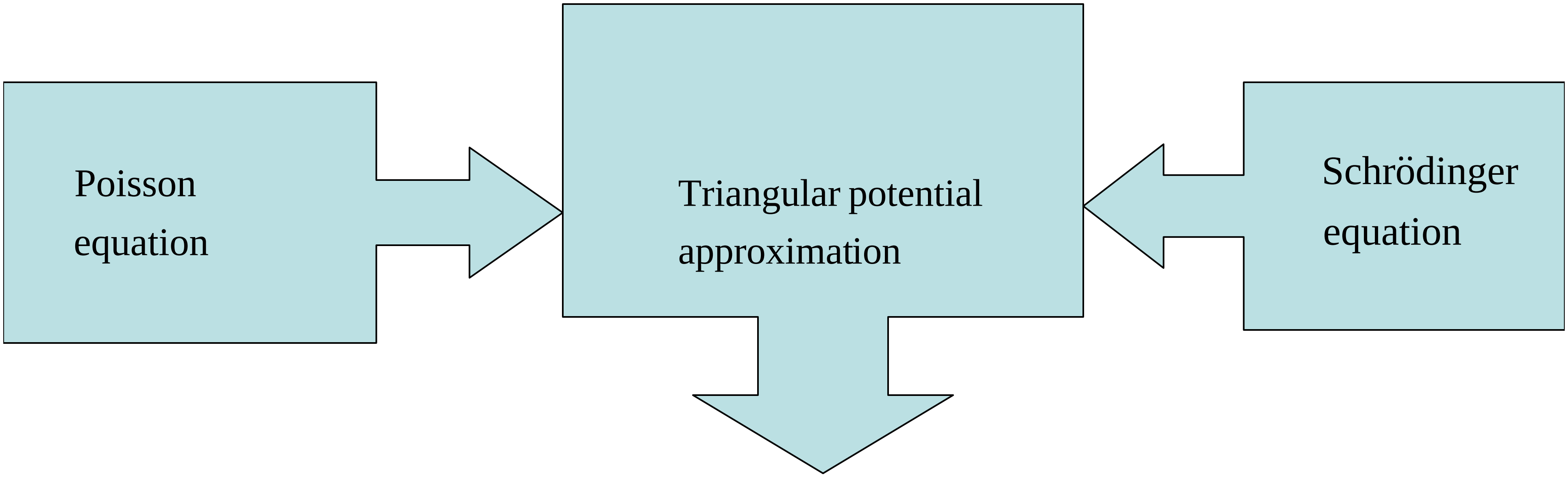
Triangular potential (continued)

- Solving the eigenvalue problem gives the ***Airy functions*** as solutions for the Schrödinger equation with energy eigenvalues

$$E_j = \left(\frac{\hbar^2}{2m^*} \right)^{1/3} \left((3/2)\pi q F_s (j + \frac{3}{4}) \right)^{2/3}$$

- Good approximation only for depletion.

Triangular potential (continued)



$$E_j = \left(\frac{\hbar^2}{2m^*} \right)^{1/3} \left((3/2)\pi q F_{seff} (j + \frac{3}{4}) \right)^{2/3}$$

- Approximation can be improved significantly at strong inversion by using the effective surface field

where $F_{seff} = \eta F_s$

WKB approach

- Improved asymptotic model for the potential:

$$U(x) = -qF_s x$$

Where $F_s = \dfrac{V_{th}\sqrt{\lambda}(\ln\lambda)^{3/2} f_s}{L_d}$,

$$f_s = \frac{\sqrt{2}\alpha_0 \coth\gamma}{\ln\lambda}, \quad \gamma = \sinh^{-1}(\alpha), \; \alpha = \alpha_0\sqrt{\ln\lambda}\,\lambda^{(1-w_s+\varphi)/2}$$

$$\alpha_0 = \sqrt{2+\varphi+\frac{\ln(\ln\lambda)}{\ln\lambda}-\frac{1}{\ln\lambda}+\frac{2}{\ln\lambda}[\ln(2\alpha_0)-\gamma]}, \quad \lambda = N_a / n_i$$

and L_d is the intrinsic Debye length

WKB approach

Poisson equation

WKB integral approximation :

$$I = \frac{\sqrt{2kT}}{c_1 \coth \gamma} \int_1^{\exp(E_j/2kT)} \frac{\sqrt{\ln(s)}}{s\sqrt{1+u^2}} ds$$

$$\text{where, } c_1 = \frac{\alpha_0 \sqrt{\lambda \ln \lambda}}{\sqrt{2} L_d}$$

Schrödinger equation

$$u = \sqrt{s^2 e^{-E_j/kT}(1-(F_0/F_s)^2) - 1 + (F_0/F_s)^2} < 1,$$

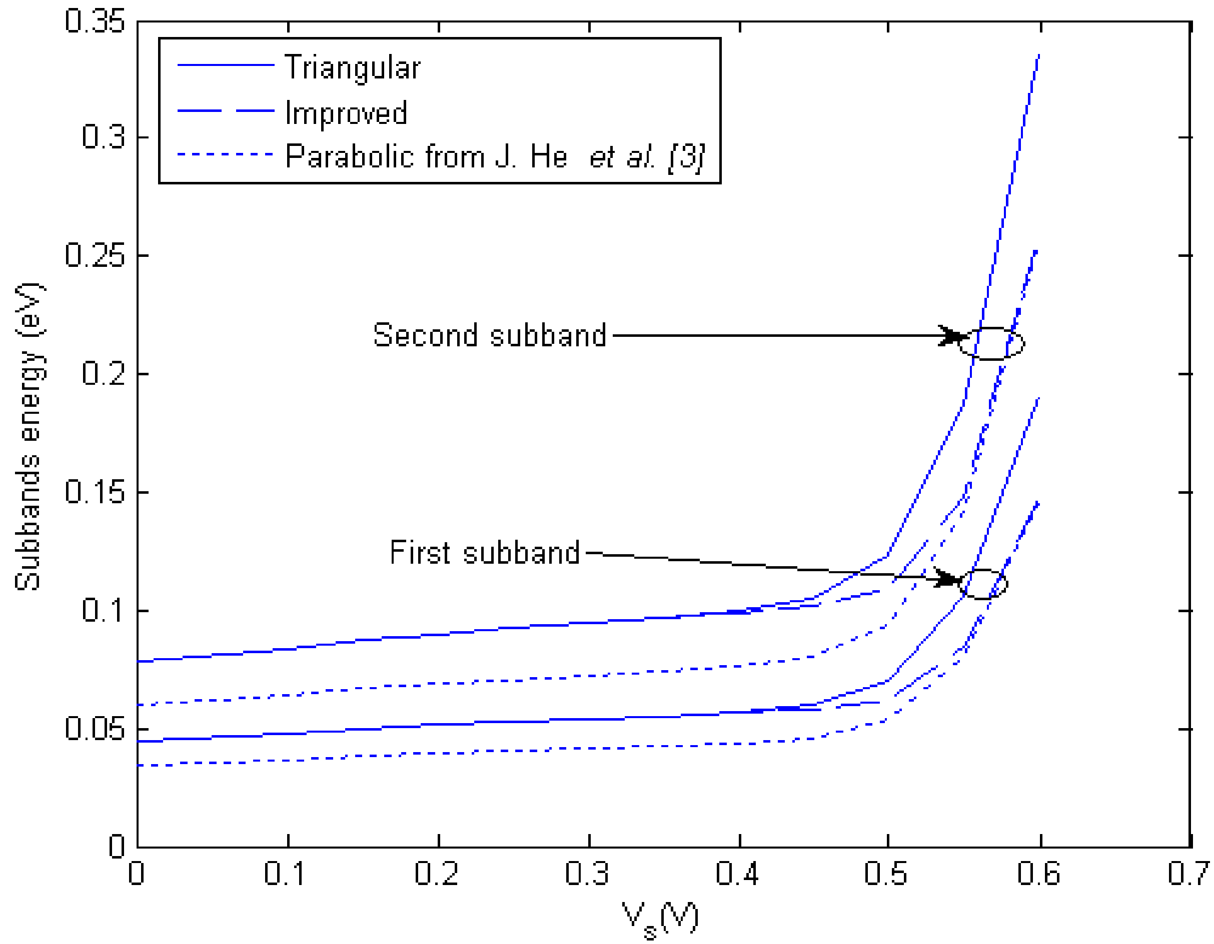
$$F_0 = \frac{\sqrt{2\lambda \ln \lambda} V_{th} \alpha_0}{L_d}.$$

First order approximation :

$$E_j = \left(\frac{\hbar^2}{2m^*}\right)^{1/3} \left((3/2)\pi q F_s (j + \frac{3}{4})\right)^{2/3}$$

Second order approximation :

$$E_j = \left(\frac{\hbar^2}{2m^*}\right)^{1/3} \left(\frac{(3/2)\pi q F_s (j + \frac{3}{4})}{(3/2) - \frac{(F_0/F_s)^2}{2}}\right)^{2/3}$$



Sub-band energy versus surface potential comparison of different analytical models from[4].

[3] J. He, M. Chan and C. Hu, "A compact model to predict quantized sub-band energy levels and inversion layer centroid of MOSFET with the parabolic potential well approximation," *Proceedings 2005 Nanotechnology Conference*, WCM, pp. 171-174, Anaheim, CA, May 8-12, 2005.

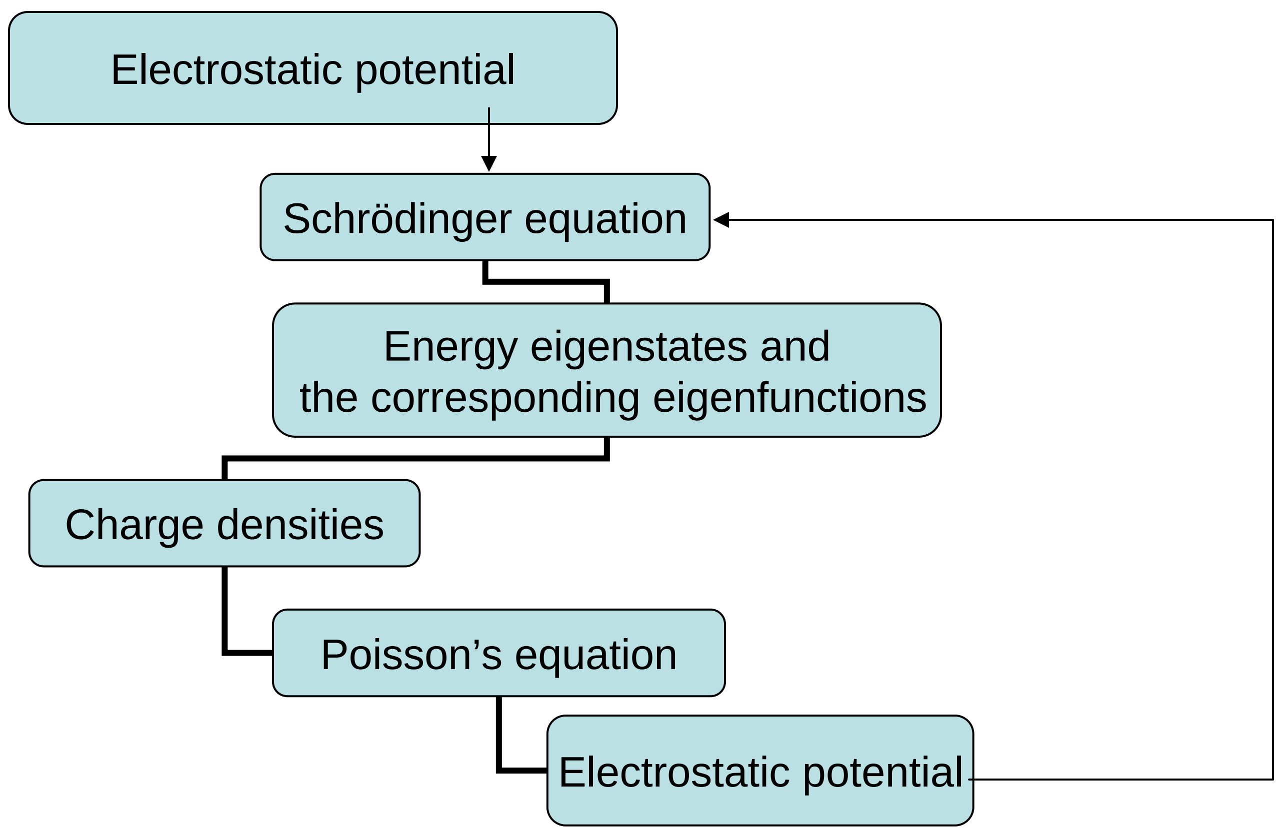
[4] E. Cumberbatch, H. Abebe, and H. Morris, "Current-voltage characteristics from an asymptotic analysis of the MOSFET equations," *J. of Engineering Mathematics*, vol. 39, pp. 25-46, 2001.

WKB approach (continued)

WKB first order integral approximation ≡ Triangular potential approximation

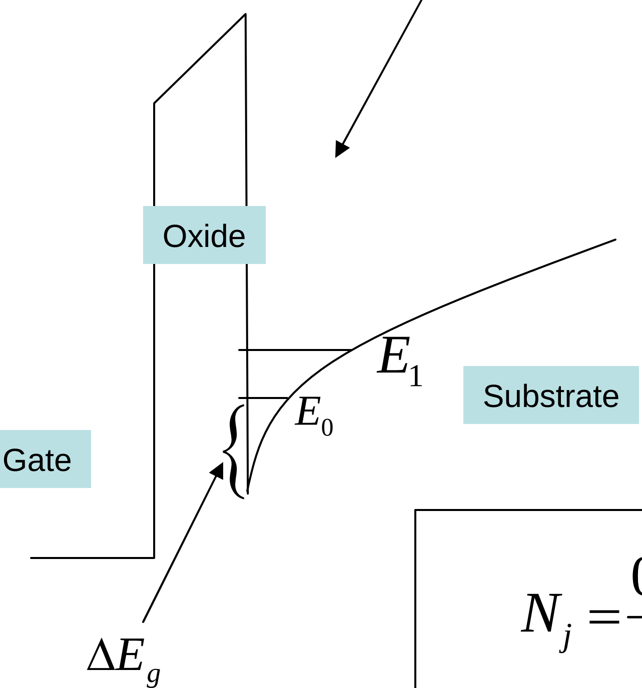
WKB second order integral approximation ≡ parabolic potential approximation

Self-Consistent Schrödinger-Poisson (SP) numerical approach



Compact model with quantum effect

Energy band profile near the interface



The electron concentration in j_{th} sub-band

$$N_j = \frac{0.38 m_e}{\pi\hbar^2} \int_{E_j}^{\infty} \frac{dE}{1+e^{(E-E_f)/kT}} = 0.38 m_e \left(\frac{kT}{\pi\hbar^2}\right) \ln\left(1+e^{(E_f-E_j)/kT}\right)$$

Carrier concentration: $n(x) = \sum_j N_j \psi_j^2(x)$

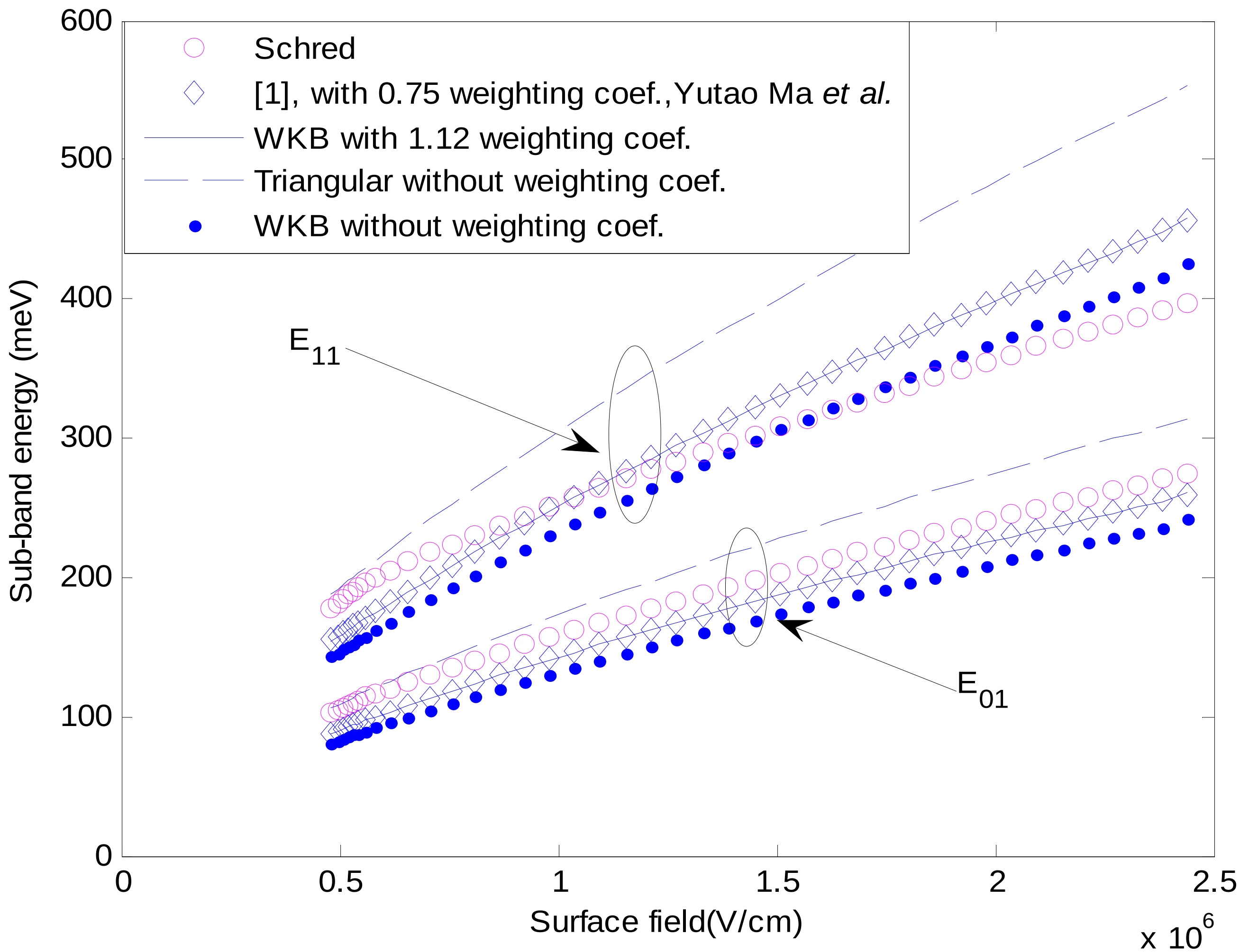
Compact model (continues)

- Quantum effect on the intrinsic charge density
- Classical:

$$n_i^c = 2\left(\frac{kT}{2\pi\hbar^2}\right)^{\frac{3}{2}} (m_h m_e)^{\frac{3}{4}} e^{-E_g/2kT)}$$

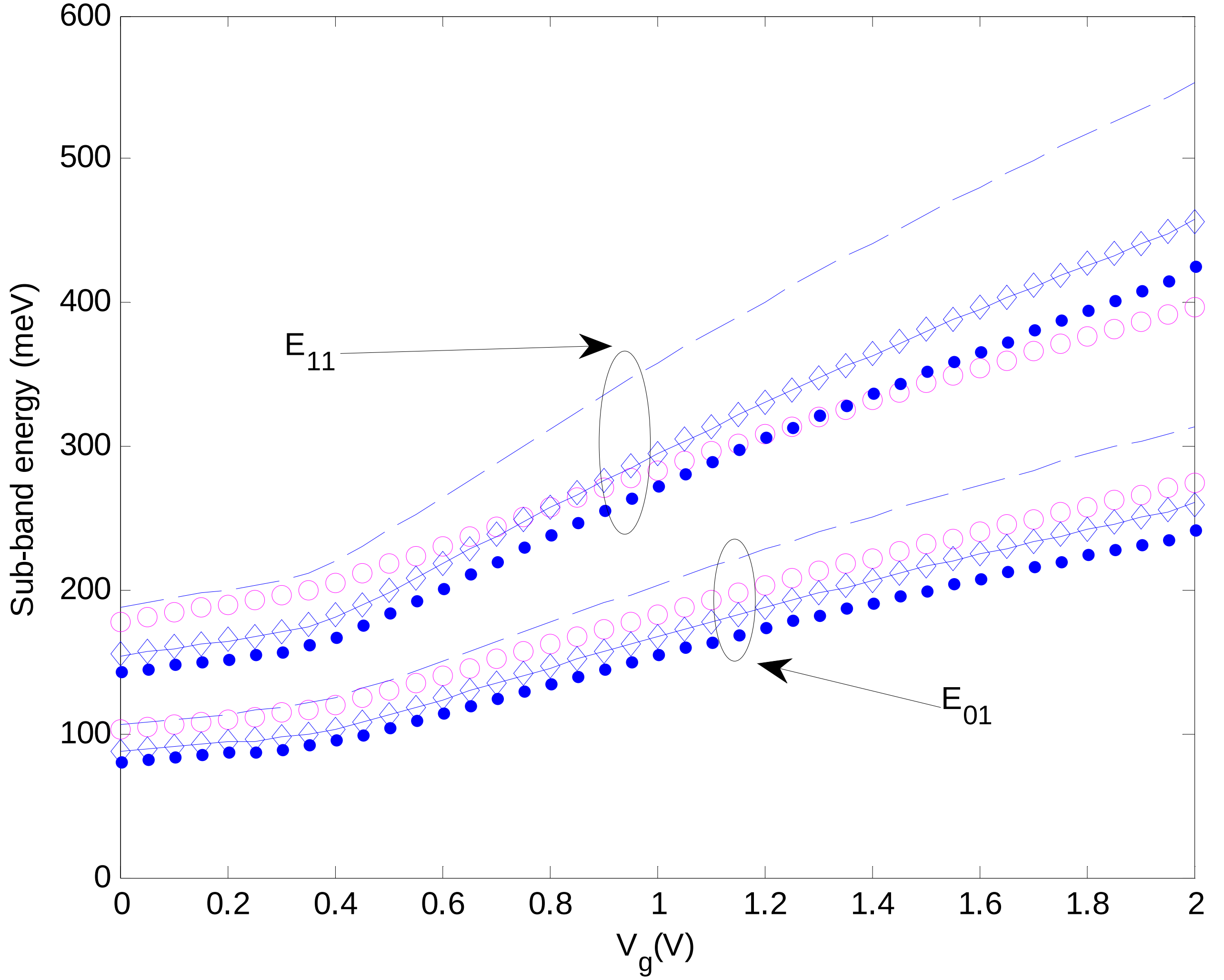
- Quantum:

$$n_i^q = e^{-\Delta E_g/2kT} n_i^c$$

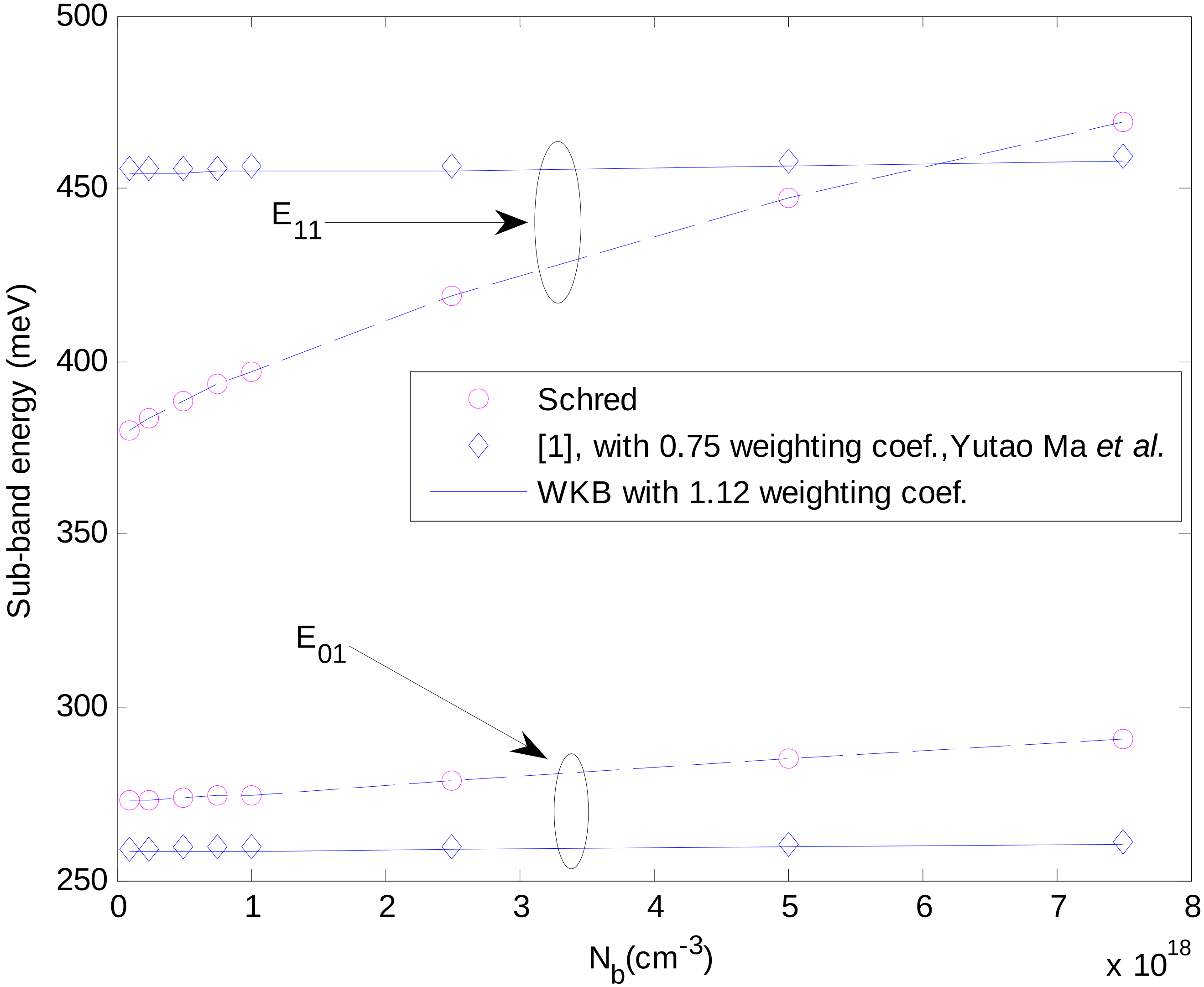


Sub-band energy versus surface field for N_b=10^{18}cm-3 and t_{ox}=2nm.

[1] Yutao Ma, Litian Liu, Zhiping Yu, and Zhijian Li, "Validity and applicability of triangular potential well approximation in modeling of MOS structure inversion and accumulation layers," *IEEE Trans. On Electron Devices*, Vol. 47, No. 9, September (2000).



Sub-band energy versus gate voltage for N_b=10^{18}cm-3 and t_{ox}=2nm.



Sub-band energy versus substrate doping for V_g=2V and t_{ox}=2nm.

Conclusion

- Triangular potential well and WKB approximation give equivalent sub-band energy results when different weighting coefficients are used in the effective surface field.
- Both Triangular potential well and WKB approximation differ in predicting the substrate doping effect on the first two lower sub-band energy levels compared to the self-consistent 1-D numerical result, SCHRED .
- Effective surface potential correction gives improvement over the original triangular potential well approximation.

Exponential approximation of the potential energy

1-D Schrödinger equation

$$\frac{d^2\zeta}{dx^2} + \frac{2m}{\hbar^2}[E - \alpha(1 - e^{-x/d})]\zeta = 0$$

$$\text{where } U = \alpha(1 - e^{-x/d}), \alpha = \lim_{x\to\infty} U(x), d = \frac{\alpha}{qF_s}$$

$$\tau^2 \frac{d^2\zeta}{d\tau^2} + \tau\frac{d\zeta}{d\tau} + [\tau^2 - (\frac{2d}{\mu}\sqrt{\alpha - E})^2]\zeta = 0$$

$$\text{where } \tau = \frac{2d}{\mu}\sqrt{\alpha}e^{-x/2d}, \mu = \frac{\hbar}{\sqrt{2m}}$$

Exponential approximation (continues)

The solution to $\zeta(\tau)$ equation can be written in terms of Bessel functions of the first kind with $v = \frac{2d}{\mu}\sqrt{\alpha - E}$:

$$\zeta(x) = C_1 J_v\left(\frac{2d}{\mu}\sqrt{\alpha}e^{-x/2d}\right)$$

With boundary conditions: $\zeta(0) = \zeta(\infty) = 0$

Exponential approximation (continues)

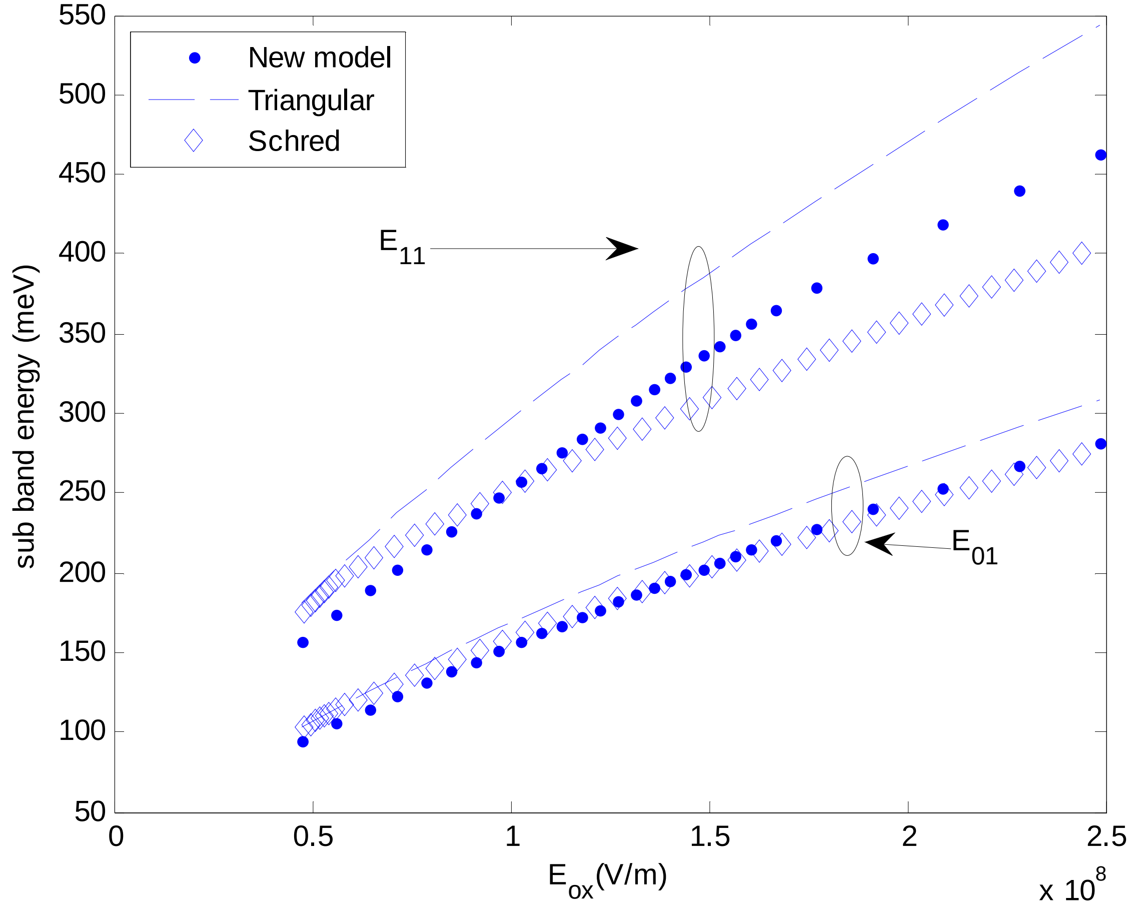
Boundary condition at x=0 ⟶ eigen value equation

$$\zeta(0) = J_v(v\sec\beta) = 0 \ \text{ where } \ \beta = \sec^{-1}\left(\sqrt{\frac{\alpha}{\alpha - E}}\right)$$

For $v >> 1$ we have asymptotic expansion (v~100):

$$J_v(v\sec\beta) \sim \frac{\cos[v(\tan\beta - \beta) - \frac{1}{4}\pi]}{\sqrt{\frac{1}{2}v\pi\tan\beta}} = 0$$

$$E_j = \alpha\sin^2\beta_j$$



Energy band level for triangular and exponential approximations compared with numerical results from SCHRED at various surface field for N_b=$10^{18}$$cm^{-3}$ and t_{ox}=2nm . The first two energy levels are shown.