Comparison of Non-Equilibrium Green's Function and Quantum-Corrected Monte Carlo Approaches in Nano MOS Simulation

H. Tsuchiya
A. Svizhenko
M. P. Anantram
M. Ogawa
T. Miyoshi

Department of Electrical and Electronics Engineering
Kobe University, Japan

NASA Ames Research Center

BACKGROUND

- **Nano-scale MOSFETs with L_{ch} < 10nm have been realized in several research laboratories.**

- **A quantum mechanical modeling of nano-scale MOSFETs involving carrier's quasi-ballistic behaviors will be indispensable.**
  - ➢ **Non-equilibrium Green's function approach (NEGF)**
  - ➢ **Quantum-corrected Monte Carlo approach (QMC)**

⬇

We present a joint study on comparison between the NEGF and QMC approaches for a nano-scale MOSFET.

Quantum-Corrected MC Approach

- Transport equation with the lowest-order quantum correction

$$\frac{\partial f}{\partial t} + \sum_{i=x,y,z} \frac{\hbar k_i}{m_i^*} \frac{\partial f}{\partial r_i} - \frac{1}{\hbar} \nabla_{\mathbf{r}} U \cdot \nabla_{\mathbf{k}} f + \underline{\frac{1}{24\hbar} (\nabla_{\mathbf{r}} \cdot \nabla_{\mathbf{k}})^3 U f} = \left(\frac{\partial f}{\partial t} \right)_C$$

- Quantum-corrected Boltzmann transport equation

$$\frac{\partial f}{\partial t} + \sum_{i=x,y,z} \frac{\hbar k_i}{m_i^*} \frac{\partial f}{\partial r_i} - \frac{1}{\hbar} \nabla_{\mathbf{r}} \left(U + \underline{U^{\mathrm{QC}}} \right) \cdot \nabla_{\mathbf{k}} f = \left(\frac{\partial f}{\partial t} \right)_C$$

- Quantum correction of potential

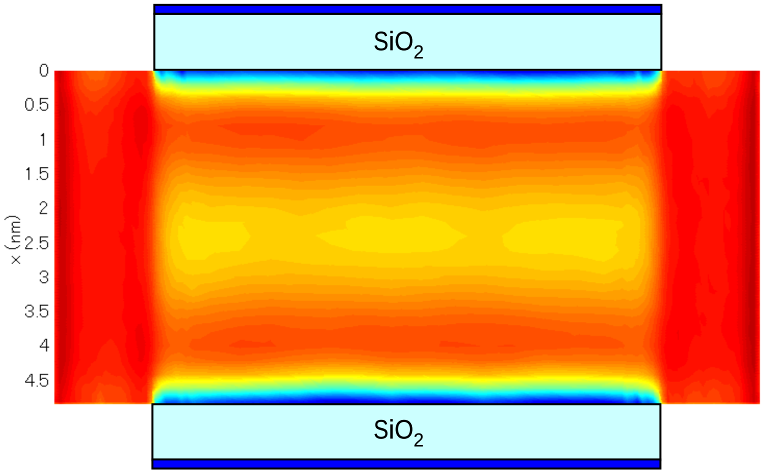
$$U^{\mathrm{QC}}(\mathbf{r}) = -\frac{\hbar^2}{12 m_x^*} \frac{\partial^2 \ln(n)}{\partial x^2} - \frac{\hbar^2}{12 m_y^*} \frac{\partial^2 \ln(n)}{\partial y^2} - \frac{\hbar^2}{12 m_z^*} \frac{\partial^2 \ln(n)}{\partial z^2}$$

- Quantum-corrected equations of motion

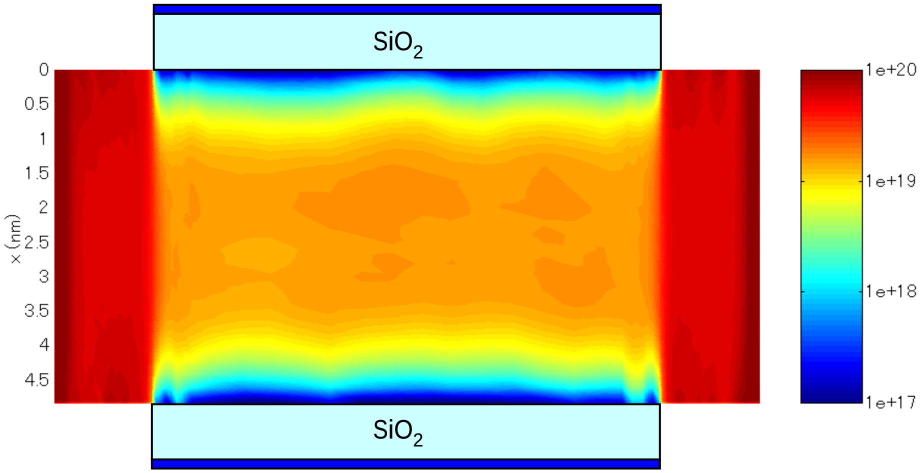
$$\frac{d\mathbf{r}}{dt} = \mathbf{v} \quad , \quad \frac{d\mathbf{k}}{dt} = -\frac{1}{\hbar} \nabla_{\mathbf{r}} \left(U + U^{\mathrm{QC}} \right)$$

Quantum-Corrected MC Simulation

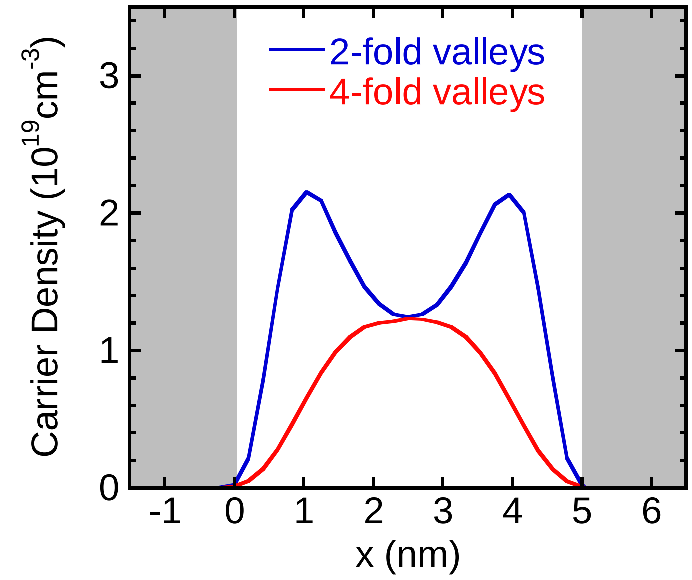
T_{Si} = 5 nm

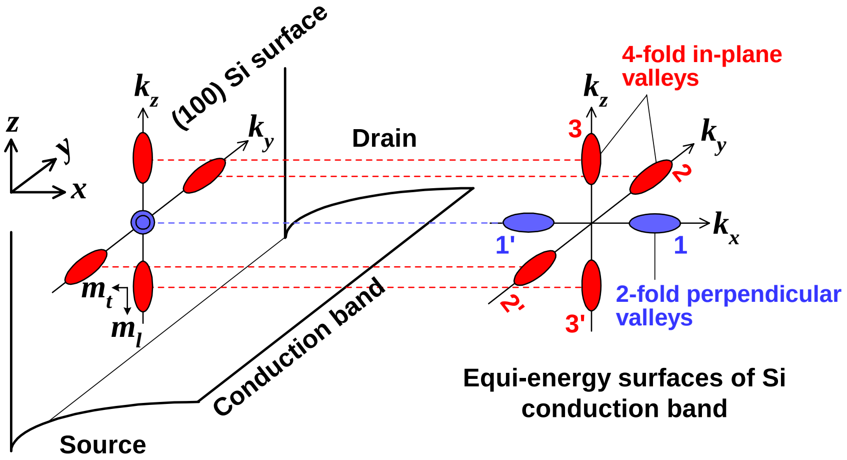


2-fold valleys



4-fold valleys





Equi-energy surfaces of Si conduction band

Quasi-2D NEGF Approach

- 1D Schrödinger equation at each cross-section

$$\left[-\frac{\hbar^2}{2m_x^\nu}\frac{d}{dx}\left(\frac{1}{m_x^\nu}\frac{d}{dx}\right)+V(x,y)\right]\psi_n(x,y)=E_n(y)\psi_n(x,y)$$

- 1D Green's function equations along channel direction

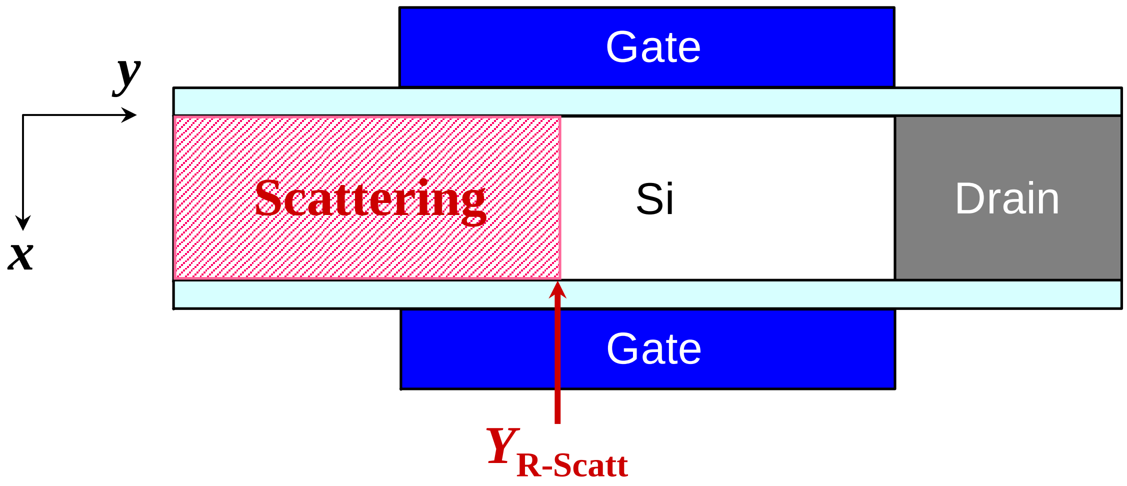
$$\left[E-\frac{\hbar^2 k_z^2}{2m_z^n}-\left(-\frac{\hbar^2}{2}\frac{d}{dy}\left(\frac{1}{m_y^n}\frac{d}{dy}\right)+E_n(y)\right)\right]G_n^r(y,y',k_z,E)$$

$$-\int dy_1 \Sigma_n^r(y,y_1,k_z,E)G_n^r(y_1,y',k_z,E)=\delta(y-y')$$

$$\left[E-\frac{\hbar^2 k_z^2}{2m_z^n}-\left(-\frac{\hbar^2}{2}\frac{d}{dy}\left(\frac{1}{m_y^n}\frac{d}{dy}\right)+E_n(y)\right)\right]G_n^{>,<}(y,y',k_z,E)$$

$$-\int dy_1 \Sigma_n^r(y,y_1,k_z,E)G_n^{>,<}(y_1,y',k_z,E)=\int dy\,\Sigma_n^{>,<}(y,y_1,k_z,E)G_n^{>,<}(y_1,y',k_z,E)$$

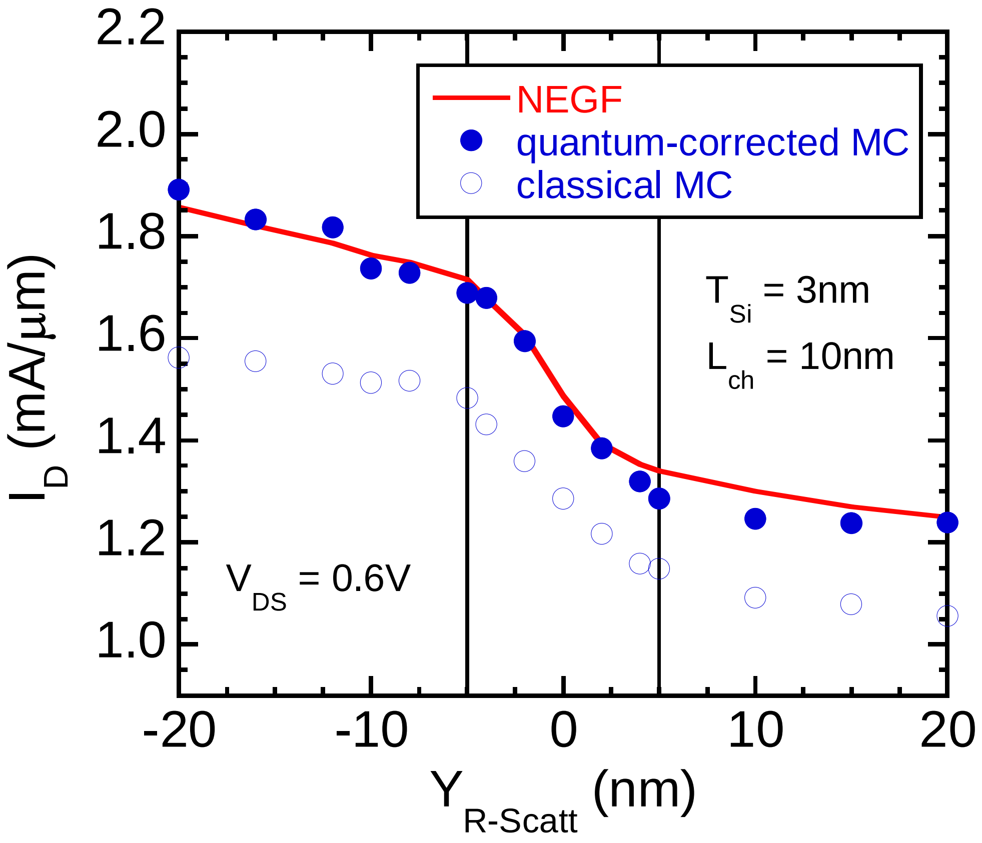
Simulation Model



- T_{Si} = 3nm
- L_{ch} = 10nm
- T_{ox} = 1.5nm
- Channel: undoped
- N_D = 10^{20} cm^{-3}
  (source and drain)

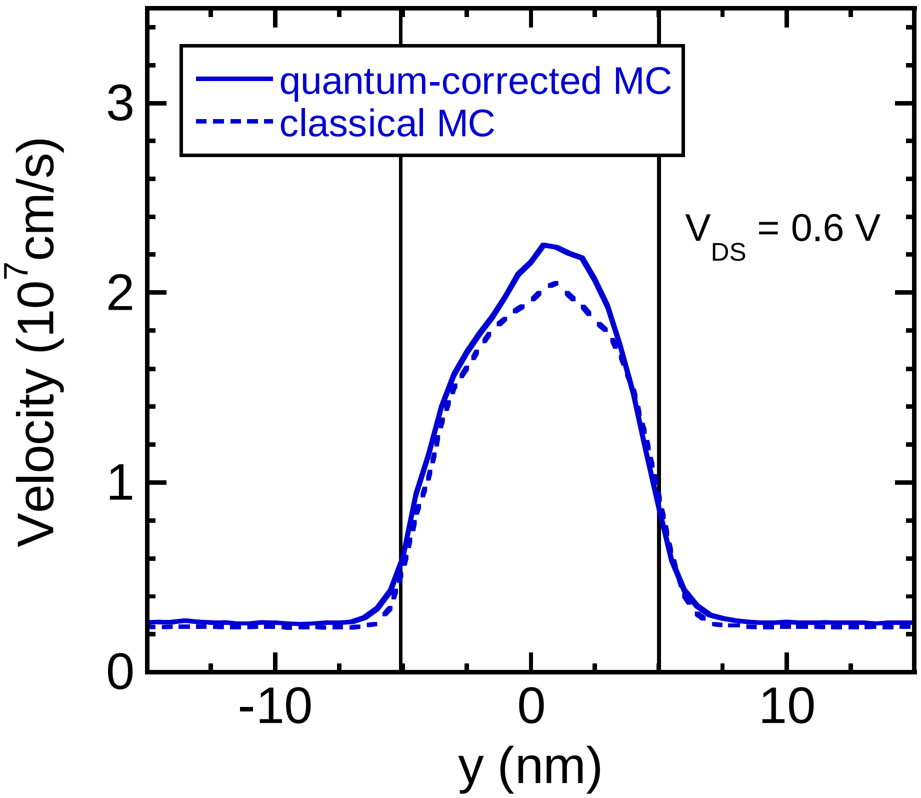
- **Drain current as a function of right boundary of scattering, $Y_{R\text{-}Scatt}$ is calculated.**
- **Only electron-phonon scattering is considered.**
- **Only the lowest quantized subbands for 2-fold and 4-fold valleys is considered in the NEGF method.**
- **Drain voltage is 0.6 V. Gate voltage is adjusted so that the injection electron density at the source edge of the channel becomes identical.**

Drain Current vs$Y_{R\text{-}Scatt}$



There is a good agreement between the NEGF and QMC results, while the classical model underestimates the drain current.

Averaged Electron Velocity Profiles



$Y_{R\text{-}Scatt}$ = 20 nm

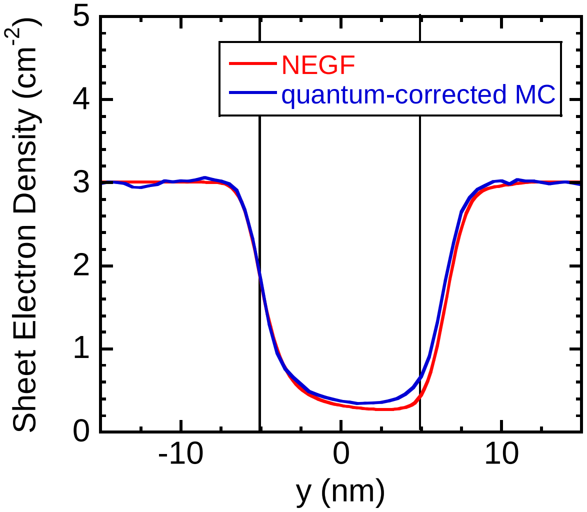
Velocity (classical) < Velocity (quantum)

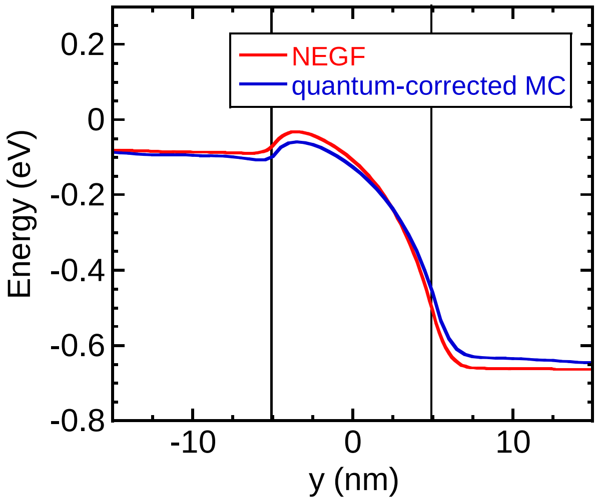
because an increase in the occupancy of the 2-fold valleys due to the energy quantizatization is not taken into account in the classical model.

Concentrations and Potentials

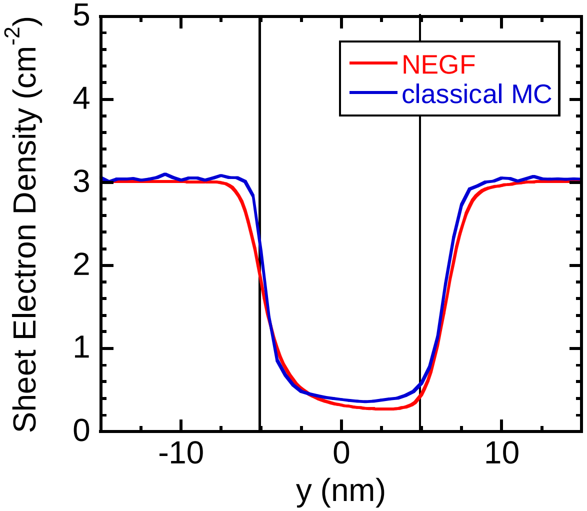
$Y_{\text{R-Scatt}} = 20\text{nm}$

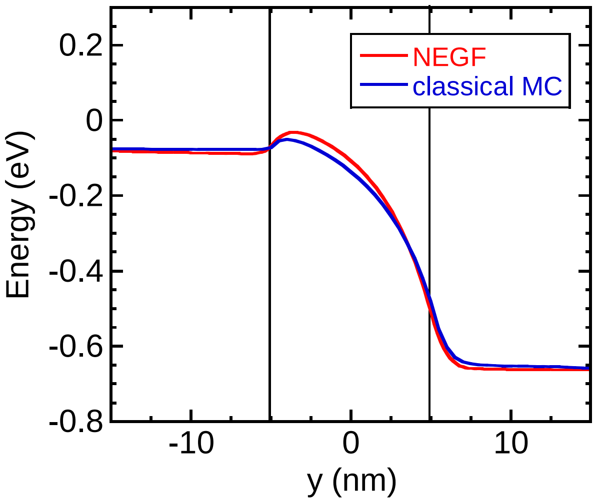
NEGF vs QMC



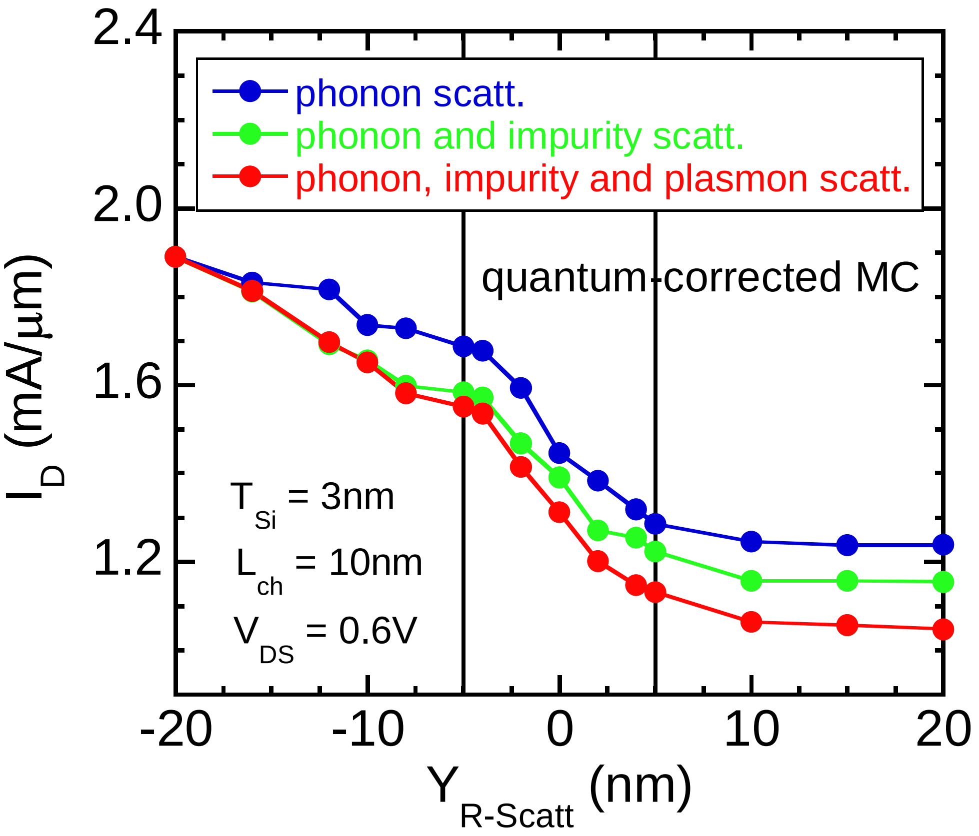


NEGF vs classical MC





Influence of Impurity and Plasmon Scatterings



- **Impurity scattering in source region**
- **plasmon scattering at drain-end of channel**

are important to estimate drain current of MOSFET.

SUMMARY

- We have found that the non-equilibrium Green's function and quantum-corrected MC approaches are equivalent in the quantum transport simulation of nano-scale MOSFETs.
    - ➢ This result may be applicable to quantum correction models such as effective potential and Bohm potential, if the subband splitting is adequately incorporated.

- We have also demonstrated that the impurity scattering in the source region and the plasmon scattering at the drain-side of the channel are important to estimate the drain current accurately.