Efficient Wigner Function Simulation for Nanowire MOSFETs and Comparison to Quantum Drift-Diffusion

O. Badami, D. Saha, S. Ganguly
CEN & Department of Electrical Engineering,
Indian Institute of Technology Bombay,
Mumbai 400076, India.
swaroop.ganguly@gmail.com.

Abstract— **In this paper, we have developed a full Quantum Device Simulator by solving the Wigner equation in the mode space for a cylindrical nanowire MOSFET. A novel and efficient numerical technique to solve the Wigner equation has been developed. It's comparison with the LU decomposition method shows that significant improvement in the simulation time is obtained. Comparison of the results obtained from the Wigner equation and Quantum Drift Diffusion method suggests that later can be continued to be used after suitable adjustments to the mobility and effective masses (across the transport). Timing comparison of the Wigner equation and QDD formalism indicates that the later is more than 200 times faster than the Wigner equation.**

Keywords- Quantum Wigner Equation, Quantum Drift Diffusion; Generalized Einstein's relatiosship ;

I. INTRODUCTION

The architecture of sub-22nm MOSFETs is evolving towards thin-body multiple-gate structures that offer superior gate control at these ultra-short channel lengths. The limit of this would be the gate-all-around nanowire transistor. In order to accurately predict the device performance in these devices it is necessary to take into account quantum effects along (Z) and across (X-Y/R-Θ) the transport direction. Different formalisms like Non-Equilibrium Green Function, Wigner function, Path-integral, Quantum Hydrodynamic and so forth have been developed to this end. All of them expectedly increase the computational load for device simulation as compared to standard drift diffusion.

In this work we present, firstly, a novel efficient scheme for the implementation of the Wigner equation along Z coupled with a Schrodinger solver in R-Θ, and Poisson for electrostatics. Secondly, we show that for situations where there are no overt quantum effects along the channel, much faster quantum drift-diffusion (QDD) simulations [1] but with generalized Einstein's relationship, can reproduce the results of the Wigner equation after some calibration. The interest in continuing to use QDD has been motivated by time needed to perform simulations.

II. FORMALISM

In this work, we solve the Schrodinger equation across the transport direction along with the Poisson equation throughout the device. Solving the Schrodinger equation allows us to work in the modes space which reduces the dimensionality of the transport equation to 1D. The transport equations are then solved in each sub-band (i.e. for each mode) and the carrier and current densities are added up (Uncoupled Mode Space Approach). The Poisson and Schrodinger equation under the cylindrical nanowire are given below (eq 1 and 2 respectively). Eq. 3, 4 and 5 are the Wigner and carrier continuity equation and drift-diffusion equations .

$$\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}\right)V = -\frac{q}{\epsilon_{SI}}(N_D-n) \tag{1}$$

$$\frac{-\hbar^2}{2}\left(\frac{1}{m^*_R}\frac{d^2}{dr^2}+\frac{1}{m^*_R}\frac{1}{r}\frac{d}{dr}+\frac{1}{m^*_\Theta}\frac{l^2}{r^2}\right)\psi - qV\psi = E_{sb}\psi \tag{2}$$

$$\frac{\hbar k}{m_z}\frac{\partial f_w}{\partial z}+\frac{1}{\hbar}\int_\infty^\infty \frac{dk'}{2\pi}\int_\infty^\infty dz'\sin\left(2z'(k-k')\right)\left(E_{sb}\left(z+\frac{z'}{2}\right)-E_{sb}\left(z-\frac{z'}{2}\right)\right)f_w = \left(\frac{\partial f_w}{\partial t}\right)_{coll} \tag{3}$$

$$\frac{dJ}{dz}=0 \tag{4}$$

$$J=\sum_{sb} n_{sb}\mu_{sb}\frac{dE_{sb}}{dz}+k_B\frac{d(n_{sb}T)}{dz} \tag{5}$$

where V is the electrostatic potential, m^*_R and m^*_Θ are the effective masses along R and Θ directions, ψ is the wave function, E_{sb} is the sub-band energy, l is the order of the Bessel function, m_z is the effective mass along the transport direction, k is wave vector, n_{sb} (m^{-1}) is the electron concentration in a particular sub-band energy and n (m^{-3}) is the total electron density. The 1D electron density obtained from the transport equation is converted into the 3D electron density (used in the Poisson equation) using the relationship $n_{3D} = n_{1D}|\psi|^2$

III. DISCRETIZATION AND SIMULATION

All the differential equations were converted to difference equation using the finite difference method. Scharfetter-Gummel discretization scheme was used for carrier continuity.

978-1-4673-5736-4/13/$31.00 ©2013 IEEE

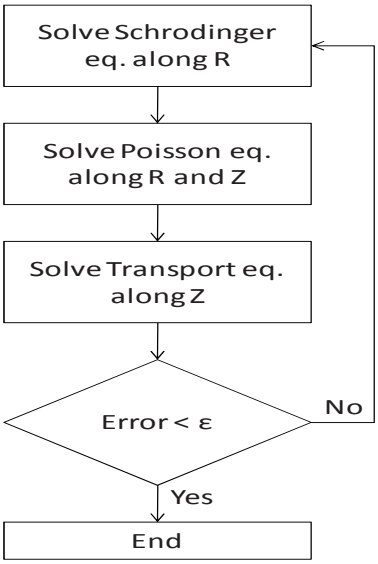

Fig.1 Flowchart for 1 bias point

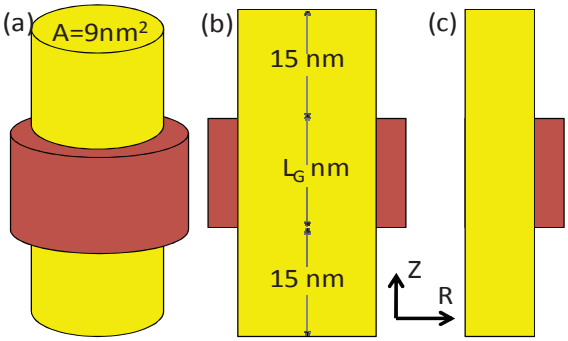

Fig.2: (a) Schematic of nanwire MOSFET (t_{ox}=0.5nm)(b) after using the angular symmetry (c) half-plane fundamental domain used for simulation

The discretization of the Wigner equation was done using the equispace meshing in both the real and reciprocal (k) space. First of all a suitable spacing in the real space was assumed, $\Delta_z$and the number real space mesh points along the transport length(L_z) was calculated using ($N_z = \frac{L_z}{\Delta_z} + 1$). The meshing in the reciprocal space was calculated using $k(j) = \frac{\pi}{\Delta_z}\left(\frac{j-0.5}{N_k} - 0.5\right)$ where j varies from 1 to N_k. The discretiztion of the derivative ($\frac{\partial f_w}{\partial z}$) in the diffusion term in the Wigner equation was done using the 3rd order upwind scheme as it offer better accuracy as shown in the Ref[2].

$$\frac{-2f_w(z-\Delta_z) - 3f_w(z) + 6f_w(z+\Delta_z) - f_w(z+2\Delta_z)}{6\Delta_z}$$
$$k < 0$$

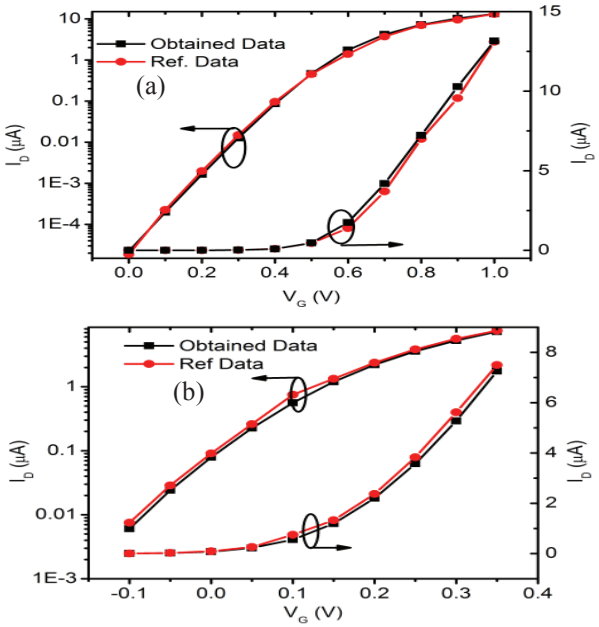

Fig.3: (a)Benchmarking of the QDD implementation with ref. data[5].(b) Benchmarking of the Wigner implementation with ref. data[6]

$$\frac{+2f_w(z+\Delta_z) + 3f_w(z) - 6f_w(z-\Delta_z) + f_w(z-2\Delta_z)}{6\Delta_z}$$
$$k > 0$$

where the argument 'k' has been suppressed in the above equations for clarity purpose. The discretization of the drift term is given by

$$\sum_{j'=1}^{N_k} V(i, j-j')\, f_w(i, j')$$

where $V(i, j-j')$ is the discretized non-local potential given by

$$V(i,j) = \frac{2}{N_k}\sum_{i'=1}^{0.5N_k} \sin\left(\frac{2\pi}{N_k} i'j\right)\left(E_{sb}(i+i') - E_{sb}(i-i')\right)$$

The scattering was taken into account using the relaxation time approximation which in the discretized form is given by

$$\frac{1}{\tau}\left(\frac{f_{eq}(z,j)}{\sum_{p=1}^{N_k} f_{eq}(z,p)}\sum_{p'=1}^{N_k} f_w(z,p') - f_w(z,j)\right)$$

where τ is the relaxation time and f_{eq} is the equilibrium Wigner distribution. Equation for current calculation for the 3rd order upwind scheme such carrier continuity is also satisfied is given by

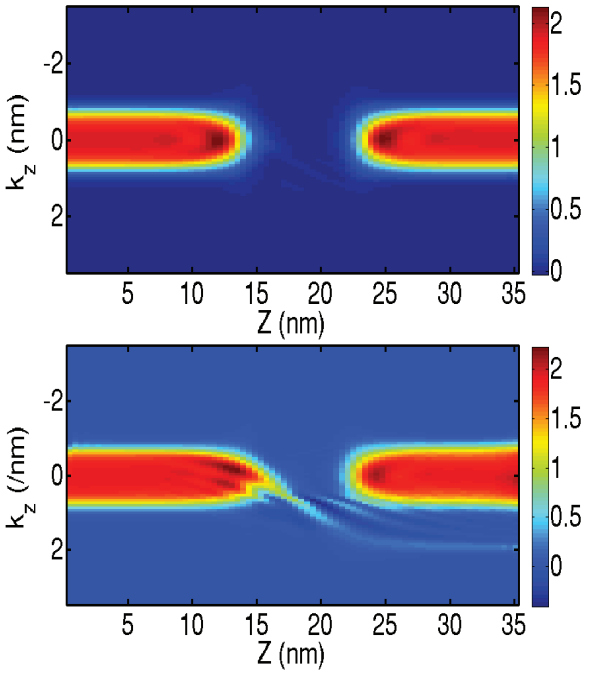

Fig.4: Cartography of the Wigner function in phase space (a) V_G=-0.1V (off-state) and (b) V_G=0.1V (on-state) and V_{DD}=0.5V, L_G=5nm. Note the increased interference between left and right moving states during increased electron flow in the on-state.

$$J_{i+0.5} = \gamma \sum_{j=1}^{N_k} k_j \begin{cases} \left(2f_w(i,j) + 5f_w(i+1,j) - f_w(i+2,j)\right); & j \le N_k/2 \\ \left(2f_w(i+1,j) + 5f_w(i,j) - f_w(i-1,j)\right); & j > N_k/2 \end{cases}$$

where $\gamma = \frac{-q\hbar\Delta_k}{12\pi m_z^*}$

Combining the discretized equation together results in equation of the form

$$[A][f_w] = [b]$$

where [b] is the column vector resulting from the boundary condtions, [f_w] is the Wigner function inside the simulation domain and [A] is the block penta-diagonal matrix of dimension N_zN_k x N_zN_k.

For the Wigner equation it was assumed that only the incoming electrons from the source and drain obey Fermi-Dirac statistics as suggested by Frensley [3]. The boundary conditions used for the Schrodinger equation, Poisson equation and carrier continuity are same as used in the Ref. 1. In this work we have used the Generalized Einstein's relationship for 1D system [4]

$$\frac{D}{\mu} = \frac{k_B T}{q}(0.7071F_{-0.5} + 2(0.1726)F_{-0.5} + \cdots) \qquad (4)$$

Fig. 1 shows the flowchart for the simulation at one bias point. Gummel iterative scheme was used for solving the equations. In order to increase the efficiency of the code we have used Fast Uncoupled Mode Space Approach (FUMS). In this technique sub-band energies are calculated by solving the

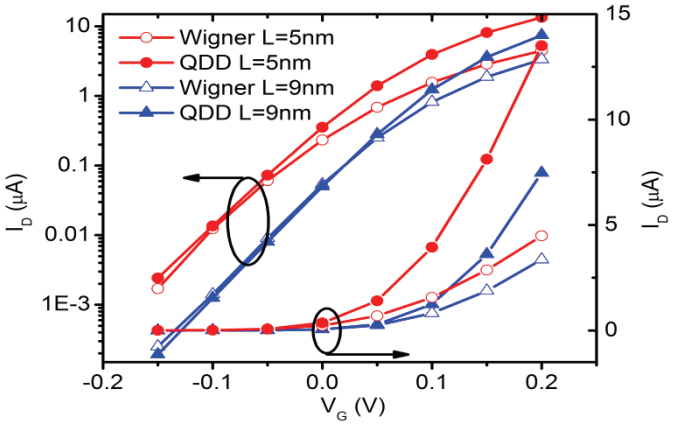

Fig.5: Comparison of I_D-V_G between QDD and Wigner equation.V_{DD} = 0.5V.

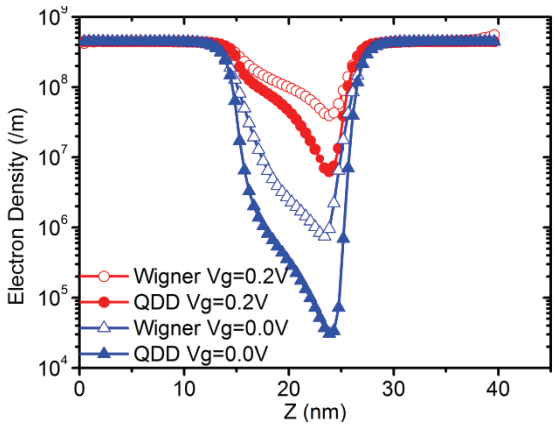

Fig.6: 1D electron density obtained by Wigner equation and QDD. V_{DD}= 0.5V

Schrodinger equation only ones and with the average (along the Z) potential and then using 1st order stationary perturbation theory[5]. The Poisson (for QDD) and carrier continuity equations were solved using the LU decomposition technique. In order to solve the system of equations for the Wigner equation we propose to use the Thomas algorithm for the block penta-diagonal matrix rather than applying LU decomposition on the entire sparse matrix, [A]. In addition to the reduction in time for simulation, memory needed to store the matrix would also be reduced. However, a disadvantage of this method is that partial pivoting can be done only on the block matrices rather than the complete matrix. The Poisson equation for the Wigner equation case was solved using the Newton's method.

Fig. 2 shows the schematic of a nanowire transistor. By exploiting the angular and inversion symmetries of the cylindrical nanowire it reduces to Fig. 2(c), the actual simulation domain. The source and drain doping in the nanowire MOSFET were assumed to be 5e19 cm^{-3} and intrinsic channel. Fig 3a shows verification of the QDD code with the reference data [5]. In this case, we have used Einstein's relationship ($\frac{D}{\mu} = \frac{k_B T}{q}$) as mentioned in the reference. For the purpose of verification (Fig. 3b) of the Wigner equation implementation we have used the data from Ref [6]. It is shown

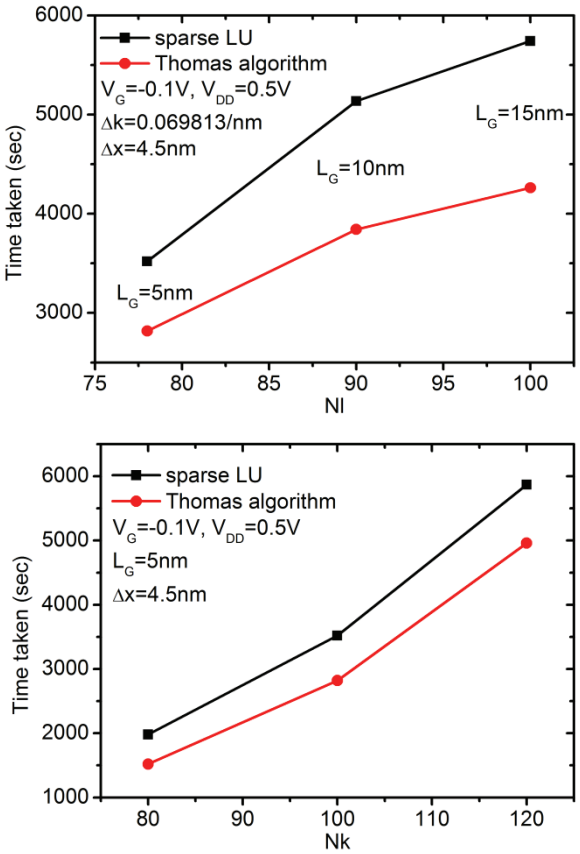

Fig.7: Comparison of time taken for one bias point simulation for different (a) Nl (channel lengths) and (b) Nk.

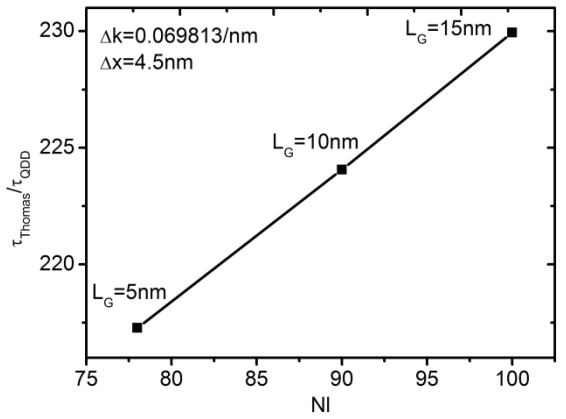

Fig. 8: Comparison of time/iteration for Wigner equation (solved with Thomas algorithm) and QDD

in [7] that for extremely scaled geometries, electron density is same irrespective of whether the cross-section is circular or square. For the purpose of simulation only one sub-band as the contribution to the electron density and hence the current from the higher sub-bands is negligible [1]. Φ_{ms}=0 was assumed in all the simulations and thus leading to depletion mode devices. Relaxation time (τ) was calculated using the relationship $\mu=q\tau/m_z$ and a constant mobility (μ) of 500 cm^2/V-sec was assumed.

IV. NUMERICAL RESULTS

Fig. 4 shows the cartography of the Wigner function under ON and OFF state. Interference between the electrons travelling from right to left and from left to right can be seen during the ON state. Fig 5 shows transfer characteristics obtained for different values of channel lengths. It can be seen that for L_G=9nm an excellent agreement in the subthreshold region was ontained indicating negligible source-drain tunneling. It is can also be seen that the mismatch between the characteristics increases with the increase in V_G. This trend can be captured using a suitable V_G dependent mobility model. Fig. 6 indicates that electron density obtained from the Wigner equation is more than that obtained from the QDD formalism. This be matched using $m_R^*$and m_θ^* as fitting parameters. Time needed for one bias point simulation using the Thomas algorithm for block penta-diagonal matrix and a straight forward LU decomposition on the sparse matrix is shown in the Fig. 7 for different values of channel length (N_Z) and N_k. It can be seen that an improvement of about 25-40% is obtained using the new method. Fig. 8 shows that QDD is more than 200 times faster than the Wigner equation .

V. CONCLUSION

In summary, we have developed a novel technique to solve the Wigner equation that is much faster than the conventional methods. A comparison of the Wigner and QDD for nanowire transistors suggests that suitably calibrated QDD can continue to be a handy design tool for these devices until quantum effects along the channel become significant through extreme length-scaling or the use of hetero-structures.

REFERENCES

[1] O.Badami, N.Kumar, D.Saha and S.Ganguly, "Quantum Drift-Diffusion and Quantum Energy Balance simulation of Nanowire MOSFETs" SISPAD 2012.

[2] Yoshihiro Yamada, Hideaki Tsuchiya and Matsuto Ogawa, "Quantum Transport Simulation of Silicon-Nanowire Transistors Based on Direct Solution Approach of the Wigner Transport Equation," IEEE Transactions on Electron Devices VOL: 56, 1396-1401, July 2009.

[3] William R. Frensley, "Wigner function model of a resonant tunneling semiconductor diode," Physical Review. B, vol. 36, no.3.

[4] OnnoW. Purbo, Daniel T.Cassidy and Stephen H. Chisholm,"Numerical model for degenerate and heterostructure semiconductor devices," Journal of Applied Physics, vol 66, no. 10.

[5] Jing Wang, "Exetension of Scharfetter-Gummel algorith, to energy balance equation,"Journal off Applied Physics, vol. 96, no. 4.

[6] Nanowires-Recent Advances, Chap 15 , Edited by Xihong Peng.

[7] Sylvain Barraud,"Phase Coherent Quantum Transport in Silicon Nanowires based on Wigner equation: Comparison with the non-Equilibrium-Green function formalism",Journal of Applied Physics, 106, 063714, 2009.