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Solution of the Space-dependent Wigner Equation Using a Particle Model

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Abstracts — The Wigner equation is well suited for numerical modeling of quantum electronic devices. In this work, the stationary, position-dependent Wigner equation is considered. Carrier scattering is described semi-classically by the Boltzmann collision operator. The development of Monte Carlo algorithms is complicated by the fact that, as opposed to the semiclassical case, the integral kernel is no longer positive semi-definite. Particle models are presented which interpret the potential operator as a generation term of numerical particles of positive and negative statistical weight. The problem arising from the avalanche of numerical particles is thereby solved for the steady state. When constructing the algorithms particular emphasis has been put on the conservation laws implied by the Wigner equation. If particles of opposite sign are generated pairwise, charge is conserved exactly. If the free-flight time is reduced such that only one particle is generated each time, then the sign of the particle weight is selected randomly, and charge is conserved only on average.

1 Introduction

At room temperature the electrical characteristics of nanoelectronic and highly down-scaled microelectronic devices are influenced simultaneously by classical and quantum transport effects. A kinetic equation suitable for describing this mixed transport regime is given by the Wigner equation. It can be formulated in a way to give the Boltzmann equation in the classical limit. The Monte Carlo (MC) method is nowadays a well established, reliable and accurate numerical method for solving the Boltzmann equation. Because of the similarity of both equations it appears very promising to develop a MC method also for the solution of the Wigner equation. Such approaches have been reported recently [1][2][3][4]. The major problem to overcome is that the Wigner potential does not represent a positive semi-definite function. This so-called negative sign problem generally demands the introduction of particles of negative statistical weight.

2 The Quantum Transport Equation

The quantum transport model is based on the generalized Wigner equation describing one electron interacting with a many-phonon system. Assuming the weak scattering limit, an equilibrium phonon system, and the mean phonon number approximation gives a system of three equations, which determines the reduced Wigner function and two auxiliary functions [5]. This model still includes effects such as collisional broadening and the intra-collisional field effect. To obtain a model more suitable for device simulation, the

classical limit is introduced in the electron-phonon interaction, which results in a Wigner equation with a Boltzmann scattering operator of the following form:

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla_r + \mathbf{F}\cdot\nabla_k\right) f_w = Q[f_w] + \Theta_w[f_w]\,. \tag{1}$$

In this equation f_w denotes the reduced electron Wigner function, $Q[f_w]$ the Boltzmann scattering operator, and $\Theta_w[f_w]$ the Wigner potential operator. The latter is defined by a convolution integral,

$$\Theta_w[f_w](\mathbf{k},\mathbf{r},t) = \int V_w(\mathbf{k}-\mathbf{k}',\mathbf{r}) f_w(\mathbf{k}',\mathbf{r},t) d\mathbf{k}' \tag{2}$$

where the kernel is given by the Wigner potential defined as

$$V_w(\mathbf{q},\mathbf{r}) = \frac{1}{(2\pi)^3 i\hbar}\int \left(V(\mathbf{r}+\tfrac{\mathbf{s}}{2}) - V(\mathbf{r}-\tfrac{\mathbf{s}}{2}) + \mathbf{s}\cdot\mathbf{F}\right)\exp(-i\mathbf{q}\cdot\mathbf{s})\,d\mathbf{s}\,. \tag{3}$$

The classical force field $\mathbf{F}(\mathbf{r})$ is introduced for convenience to obtain a Liouville operator of a form compatible with the classical Boltzmann equation [2]. However, terms in (1) and (3) related to the force field cancel each other, such that the choice of this field is arbitrary and has no effect on the solution.

Because the Wigner potential assumes positive and negative values, it cannot be directly used as a probability density. However, because of its antisymmetry with respect to $\mathbf{q}$ the Wigner potential can be reformulated in terms of one positive function V_w^+ [4],

$$V_w^+(\mathbf{q},\mathbf{r}) = \max_{\mathbf{q}}(0, V_w(\mathbf{q},\mathbf{r}))\,, \tag{4}$$

$$V_w(\mathbf{q},\mathbf{r}) = V_w^+(\mathbf{q},\mathbf{r}) - V_w^+(-\mathbf{q},\mathbf{r})\,. \tag{5}$$

The Liouville operator in (1) is now expressed as a total time derivative over a classical trajectory $\mathbf{K}(t),\mathbf{R}(t)$. Writing the operators on the right hand side explicitly gives

$$\left[\frac{\mathrm{d}}{\mathrm{d}t} + (\lambda+\alpha)\right] f_w(\mathbf{k},\mathbf{r},t) = \int [S(\mathbf{k}',\mathbf{k}) + \alpha\,\delta(\mathbf{k}'-\mathbf{k})] f_w(\mathbf{k}',\mathbf{r},t)\,d\mathbf{k}' + \int V_w^+(\mathbf{q},\mathbf{r})\,[f_w(\mathbf{k}-\mathbf{q},\mathbf{r},t) - f_w(\mathbf{k}+\mathbf{q},\mathbf{r},t)]\,d\mathbf{q}\,. \tag{6}$$

The three characteristic rates in this equation are the semiclassical scattering rate, $\lambda(\mathbf{k}) = \int S(\mathbf{k},\mathbf{k}')\,d\mathbf{k}'$, a self-scattering rate to be determined later, $\alpha(\mathbf{k},\mathbf{r}) \geq 0$, and a rate associated with the Wigner potential, $\gamma(\mathbf{r}) = \int V_w^+(\mathbf{q},\mathbf{r})\,d\mathbf{q}$. These rates are the normalization factors needed to define the following conditional probability distributions:

$$s(\mathbf{k}|\mathbf{k}') = \frac{S(\mathbf{k}',\mathbf{k})}{\lambda(\mathbf{k}')}\,, \qquad w(\mathbf{k}|\mathbf{k}') = \frac{V_w^+(\mathbf{k}-\mathbf{k}')}{\gamma}\,, \qquad w^*(\mathbf{k}|\mathbf{k}') = w(\mathbf{k}'|\mathbf{k})\,. \tag{7}$$

For the sake of brevity writing the $\mathbf{r}$-dependence of these distributions is omitted. Defining the kernel

$$\Gamma(\mathbf{k}|\mathbf{k}') = \frac{\lambda}{\mu}\,s(\mathbf{k}|\mathbf{k}') + \frac{\alpha}{\mu}\,\delta(\mathbf{k}'-\mathbf{k}) + \frac{\gamma}{\mu}\,[w(\mathbf{k}|\mathbf{k}') - w^*(\mathbf{k}|\mathbf{k}')]\,, \tag{8}$$

where $\mu = \lambda + \alpha$, allows (6) to be written as

$$\left[\frac{\mathrm{d}}{\mathrm{d}t} + \mu(\mathbf{k})\right] f_w(\mathbf{k}, \mathbf{r}, t) = \int \Gamma(\mathbf{k}|\mathbf{k}')\mu(\mathbf{k}') f_w(\mathbf{k}', \mathbf{r}, t) d\mathbf{k}' \,. \tag{9}$$

Note that the Wigner equation conserves charge, as can be easily seen by integrating (1) in $\mathbf{k}$-space. A continuity equation without source term is obtained, because the integrals of the scattering operator and the potential operator vanish, $\int Q[f_w](\mathbf{k}) d\mathbf{k} = 0$ and $\int \Theta_w[f_w](\mathbf{k}) d\mathbf{k} = 0$. Consequently, also the kernel (8) conserves charge, $\int \Gamma(\mathbf{k}|\mathbf{k}') d\mathbf{k} = 1$.

The integral form of the Wigner equation is derived from (9) in the same way as the integral form of the Boltzmann equation [6][7]. The propagation of particles in forward time direction is governed by theh adjoint equation:

$$\begin{aligned} g_w(\mathbf{k}, \mathbf{r}, t) &= g_0(\mathbf{k}, \mathbf{r}, t) + \\ &+ \int_t^\infty d\tau \int d\mathbf{k}' g_w(\mathbf{K}(\tau), \mathbf{R}(\tau), \tau) \exp\left(-\int_t^\tau \mu(\mathbf{K}(y)) dy\right) \Gamma(\mathbf{k}'|\mathbf{k}) \mu(\mathbf{k}) \Theta_D(\mathbf{r}) \,. \end{aligned} \tag{10}$$

Θ_D denotes the indicator function of the simulation domain D. The initial conditions for the phase space trajectory are $\mathbf{K}(t) = \mathbf{k}'$, $\mathbf{R}(t) = \mathbf{r}$.

3 Particle Models

In analogy with the Boltzmann equation [6] each term of the Neumann series of (10) describes a sequence of consecutive free flight and scattering events. A transition consisting of a free flight with initial state $\mathbf{k}_i$ at time t_i, and a scattering process to the final state $\mathbf{k}_f$ at time t_f is described by

$$P(\mathbf{k}_f, t_f|\mathbf{k}_i, t_i) = \Gamma(\mathbf{k}_f|\mathbf{K}_i(t_f))\ \mu(\mathbf{K}_i(t_f)) \exp\left(-\int_{t_i}^{t_f} \mu(\mathbf{K}_i(\tau)) d\tau\right). \tag{11}$$

In a MC simulation the time of the next scattering event, t_f, is generated from an exponential distribution. Then a transition from the trajectory end point $\mathbf{K}_i(t_f)$ to the final state $\mathbf{k}_f$ is realized using the kernel Γ. In contrast to the classical case, P does not represent a probability because Γ is not positive semi-definite. In the following different variants of generating the final state $\mathbf{k}_f$ from the kernel Γ will be discussed.

3.1 Instable Methods

A straightforward idea would be to use the absolute value of Γ as a transition probability. Practically it is more convenient to use the absolute values of the components of Γ, giving a transition probability of the form

$$p(\mathbf{k}_f|\mathbf{k}') = \frac{\lambda}{\nu} s(\mathbf{k}_f|\mathbf{k}') + \frac{\alpha}{\nu} \delta(\mathbf{k}_f - \mathbf{k}') + \frac{\gamma}{\nu} w(\mathbf{k}_f|\mathbf{k}') + \frac{\gamma}{\nu} w^*(\mathbf{k}_f|\mathbf{k}'), \tag{12}$$

where the normalization factor is $\nu = \lambda + \alpha + 2\gamma$.

Method I1: The free-light time is generated from the exponential distribution appearing in (11),

$$p_t(t_f|t_i,\mathbf{k}_i) = \mu(\mathbf{K}_i(t_f))\exp\left(-\int_{t_i}^{t_f}\mu(\mathbf{K}_i(\tau))d\tau\right). \tag{13}$$

For the sake of brevity the state at the end of the free flight is labeled $\mathbf{k}' = \mathbf{K}_i(t_f)$ in the following. To generate the final state $\mathbf{k}_f$, one of the four terms in (12) is selected with the associated probabilities λ/ν, α/ν, γ/ν, and γ/ν, respectively. Clearly, these probabilites sum up to one. If classical scattering is selected, $\mathbf{k}_f$ is generated from s. If self-scattering is selected, the state does not change and it holds $\mathbf{k}_f = \mathbf{k}'$. If the third or fourth term are selected, the particle state is changed by scattering from the Wigner potential and $\mathbf{k}_f$ is selected from w or w^*, respectively. The particle weight has to be multiplied by the ratio

$$\frac{\Gamma}{p} = \pm\left(1+\frac{2\gamma}{\lambda+\alpha}\right), \tag{14}$$

where the minus sign applies if $\mathbf{k}_f$ has been generated from w^*. For instance, for the typical case of the classical scattering rate λ being less than the Wigner scattering rate γ, the self-scattering rate α can be chosen such that $\lambda+\alpha=\gamma$. Then the multiplier (14) evaluates to ± 3.

The drawback of this method is that the magnitude of the weight increases at each scattering event by the multiplier (14). The growth rate of the weight can be estimated for the case of constant coefficients γ and μ. Since free flight times are generated with rate μ, the mean free flight time will be $1/\mu$. During a given time interval t on average $n = \mu t$ scattering events will occur. The total weight is then estimated asymptotically for $t \gg 1/\mu$ as:

$$|W(t)| = \left(1+\frac{2\gamma}{\mu}\right)^n = \left(1+\frac{2\gamma t}{n}\right)^n \simeq \exp(2\gamma t) \tag{15}$$

This expression shows that the growth rate is determined by the Wigner scattering rate γ independently of the classical and the self-scattering rates.

Method I2: The same time-dependence of the particle weight is obtained for a similar MC algorithm. Again the transition rate (12) is used, but now the free flight time is generated with rate ν and not with μ. In this case (11) can be rewritten as

$$\begin{aligned} P(\mathbf{k}_f,t_f|\mathbf{k}_i,t_i) = {} & \frac{\Gamma(\mathbf{k}_f|\mathbf{k}')\,\mu(\mathbf{k}')}{p(\mathbf{k}_f|\mathbf{k}')\,\nu(\mathbf{k}')}p(\mathbf{k}_f|\mathbf{k}') \\ & \times \nu(\mathbf{k}')\exp\left(-\int_{t_i}^{t_f}\nu(\mathbf{K}_i(\tau))d\tau\right)\exp\left(2\int_{t_i}^{t_f}\gamma(\mathbf{R}_i(\tau))d\tau\right) \end{aligned} \tag{16}$$

The exponential distribution and the distribution p are used to generate t_f and $\mathbf{k}_f$, respectively. The remaining terms form the factor, by which the particle weight changes during one free flight. Because of $(\Gamma\mu)/(p\nu) = \pm 1$ the multiplier for the i-th free flight evaluates to

$$m_i = \pm\exp\left(2\int_{t_i}^{t_{i+1}}\gamma(\mathbf{R}_i(\tau))d\tau\right) \tag{17}$$

The total weight after n free flights finally grows as a function of the whole path integral over $\gamma(\mathbf{R}(\tau))$:

$$|W(t_n)| = \prod_{i=0}^{n-1} |m_i| = \exp\left(2\int_0^{t_n} \gamma(\mathbf{R}(\tau))d\tau\right) \tag{18}$$

This result generalizes (15) for a position-dependent γ. The growth rate 2γ is equal to the L_1 norm of the Wigner potential.

Using these methods it has been demonstrated that tunneling can be treated numerically by means of a particle model [3]. However, because of the exponentially increasing particle weight at the very short time scale $(2\gamma)^{-1}$, application of this algorithm turned out to be restricted to single-barrier tunneling and small barrier heights only. The methods of this section can be useful for devices where quantum effects are weak, and the potential operator is a small correction to the otherwise classical transport equation.

3.2 Pair Generation Methods

To solve the problem of increasing particle weight one can split the particle. In this way an increase in particle weight is transformed to an increase in particle number. A stable MC algorithm is constructed by adding a measure for removing numerical particles. Particles of opposite sign and sufficiently small distance in phase space can be annihilated, allowing the number of numerical particles to be kept below desired bounds.

The basic idea of splitting is refined so as to avoid fractional weights. Different interpretations of the kernel are presented that conserve the magnitude of the particle weight. Choosing the initial weight to be $+1$ all generated particles will have weight $+1$ or -1. This is achieved by interpreting the potential operator in (6) as a generation term of positive and negative particles. We consider the kernel

$$\Gamma(\mathbf{k}_f|\mathbf{k}') = \frac{\lambda}{\mu}\, s(\mathbf{k}_f|\mathbf{k}') + \frac{\alpha}{\mu}\,\delta(\mathbf{k}_f - \mathbf{k}') + \frac{\gamma}{\mu}\left[w(\mathbf{k}_f|\mathbf{k}') - w^*(\mathbf{k}_f|\mathbf{k}')\right] \tag{19}$$

If the Wigner scattering rate γ is larger than the classical scattering rate λ, the self-scattering rate α has to be chosen large enough to satisfy the inequality $\gamma/\mu \leq 1$. Typical choices are $\mu = \mathrm{Max}(\lambda, \gamma)$ or $\mu = \lambda + \gamma$. These expressions also hold for the less interesting case $\gamma < \lambda$, where quantum interference effects are less important than classical scattering effects.

As in the classical MC method, the distribution of the free flight duration is given by the exponential distribution (13). At the end of a free flight the complementary probabilities $p_s = \lambda/\mu$ and $1 - p_s = \alpha/\mu$ are considered. With probability p_s classical scattering is selected. The final state is generated from s. The complementary event is self-scattering. In addition, with probability $p_w = \gamma/\mu$ a pair of particle states is generated from the distributions w and w^*. The multiplier of the weight is $+1$ for a state generated from one of first three terms, and -1 for a state generated from w^*. Therefore, the magnitude of the initial particle weight is conserved.

Method G1: In the following we discuss the case $\gamma > \lambda$, where quantum effects are dominant. We begin with the smallest possible value for μ: $\mu = \mathrm{Max}(\lambda, \gamma) = \gamma$. Because $p_w = \gamma/\mu = 1$, a particle pair is generated after each free flight as shown in Fig. 1. At the same instances classical or self-scattering events occur. In Fig. 1 and the following

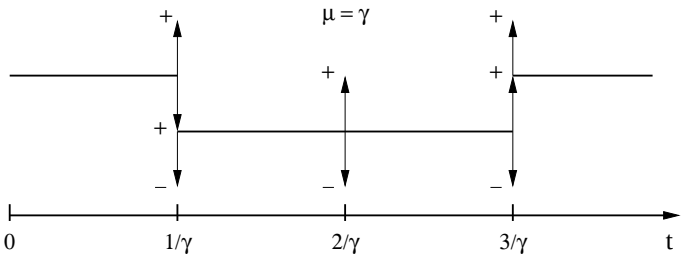

Figure 1: Trajectory of a sample particle resulting from Method G1.

figures only the trajectory of one sample particle is shown and not the whole cascade of trajectories of the generated particles.

Method G2: Choosing the self-scattering rate to be $\alpha = \gamma$ the kernel can be regrouped as

$$\Gamma(\mathbf{k}_f|\mathbf{k}') = \frac{\lambda}{\mu}\, s(\mathbf{k}_f|\mathbf{k}') + \big(1 - \frac{\lambda}{\mu}\big)\big(\delta(\mathbf{k}_f - \mathbf{k}') + w(\mathbf{k}_f|\mathbf{k}') - w^*(\mathbf{k}_f|\mathbf{k}')\big) \tag{20}$$

With probability $p_s = \lambda/\mu$ classical scattering is selected. Otherwise, a self-scattering event and a pair generation event occur. In this algorithm classical scattering and pair generation cannot occur at the same time, as shown in Fig. 2. Compared to Method G1, the average free flight time is now reduced, because μ has been increased from γ to $\lambda+\gamma$.

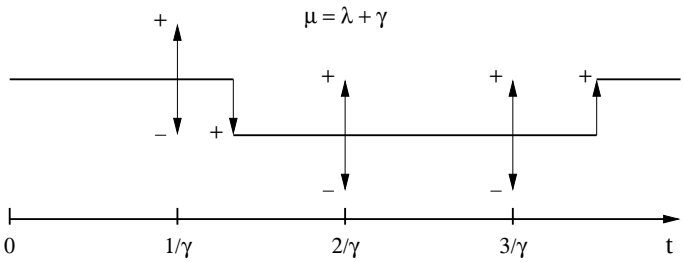

Figure 2: Trajectory of a sample particle resulting from Method G2.

3.3 Single Particle Generation Methods

The idea of this method is to further reduce the free flight time. We rewrite the kernel as

$$\Gamma(\mathbf{k}_f|\mathbf{k}') = \frac{\lambda}{\mu}\, s(\mathbf{k}_f|\mathbf{k}') + \frac{\alpha}{\mu}\,\delta(\mathbf{k}_f - \mathbf{k}') + \frac{2\gamma}{\mu}\left[\frac{1}{2}w(\mathbf{k}_f|\mathbf{k}') - \frac{1}{2}w^*(\mathbf{k}_f|\mathbf{k}')\right]. \tag{21}$$

In this case the self-scattering rate α has to be chosen large enough to satisfy the inequality $2\gamma/\mu \leq 1$. Typical choices are $\mu = \mathrm{Max}(\lambda, 2\gamma)$ and $\mu = \lambda+2\gamma$. As in Method G1 classical scattering is selected with probability $p_s = \lambda/\mu$, whereas the the complementary event is self-scattering. In addition, with probability $p_w = 2\gamma/\mu$ particle generation is selected.

If selected, with equal probability either the distribution w or w^* is chosen to generate the final state $\mathbf{k}_f$. If w^* has been chosen the weight is multiplied by -1.

Method G3: Assuming $\gamma > \lambda/2$ and $\mu = 2\gamma$ gives $p_w = 1$. Therefore, after each free flight either a positive or negative particle is generated, as depicted in Fig. 3. At the same instances classical or self-scattering events occur.

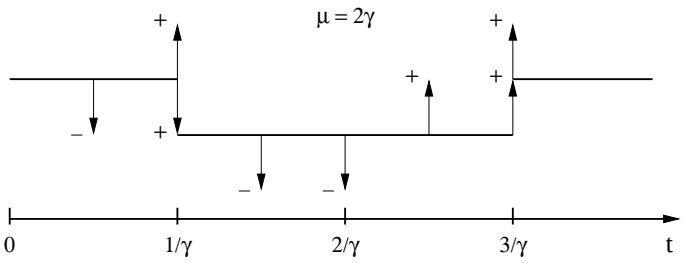

Figure 3: Trajectory of a sample particle resulting from Method G3.

Note that in Method G3 ($\mu = 2\gamma$) the free flight time is reduced by a factor two compared to Method G1 ($\mu = \gamma$), which means that now the kernel is applied twice as frequently. In Method G3 single particles are generated at a rate of 2γ, whereas in Method G1 particle pairs are generated at half of this rate.

Method G4: In this method we set $\alpha = 2\gamma$ and obtain $\mu = \lambda + 2\gamma$. In analogy with Method G2 classical scattering and particle generation are now complementary events. Fig. 4 indicates that these two types of events occur at different times. From all methods discussed above this method uses the shortest free flight time.

From a numerical point of view Method G1 and Method G2 have the advantage that they exactly conserve charge as they generate particles pairwise with opposite sign. Method G3 and Method G4 generate only one particle each time. Because the sign of the weight is selected randomly, charge is conserved only on average. Simulation experiments, however, have shown that the quality of the pseudo random number generator is good enough to generate almost equally many positive and negative particles even during long simulation times, such that the small difference of net generated particles has no visible effect on the solution.

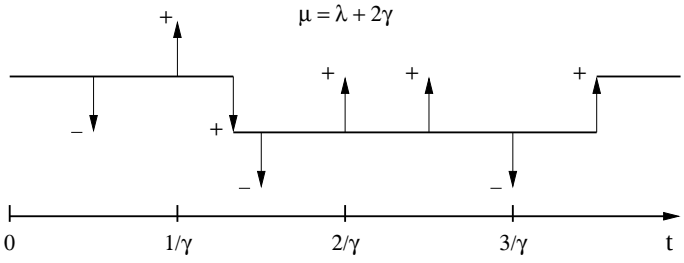

Figure 4: Trajectory of a sample particle resulting from Method G4.

3.4 Other Methods

In Method G1 to Method G4 the weight of the generated particles is ± 1, because the generation rate used equals 2γ. If a generation rate larger than 2γ or a fixed time-step less than $1/2\gamma$ were used, the magnitude of the generated weight would be less than 1. This approach has been followed in [1], where the resulting fractional weights are termed affinities. On the other hand, a generation rate less than 2γ would result in an under-sampling of the physical process. The magnitude of the generated weights would be generally larger than 1.

3.5 Particle Annihilation

The discussed particle models are instable, because either the particle weight or the particle number grows exponentially in time. A stable MC algorithm can be obtained by combining one of the particle generation methods with a method to control the particle number. One can assume that two particles of opposite weight and a sufficiently small distance in phase space annihilate each other. In an ensemble MC method a particle removal step should be performed at given time steps. During the time step the ensemble is allowed to grow to a certain limit, then particles are removed and the initial size of the ensemble is restored. In this work the problem has been solved for the stationary transport problem. In the algorithm the trajectory of only one sample particle is followed, whereas other numerical particles are temporarily stored on a state space grid. Due to the opposite sign, particle weights annihilate to a large extent in the cells of the grid. The total residual weight in each cell has to be minimized, as it represents a measure for the numerical error of the method [8].

4 Results

A resonant tunneling diode (RTD) has been studied. The characteristic parameters are a barrier height of $E_b = 0.47\,\mathrm{eV}$, a barrier width of 3 nm, and a well width of 4 nm. The Wigner potential $V_w^+(k_x, x)$ is discretized using $N_k = 1200$ equidistant k_x points and $\Delta x = 0.5\,\mathrm{nm}$ spacing in the x-direction. A coherence length of $L_c = 60\mathrm{nm}$ is assumed. The annihilation mesh consists of 480 points in the longitudinal and 120 points in the perpendicular momentum direction, and the real space coordinate is disretized using $\Delta x = 0.5\,\mathrm{nm}$.

Fig. 5 shows the electron concentration profile in the device obtained using Method G2. At the resonance voltage of 1.2 V the concentration in the quantum well is considerably higher than in the off-resonance condition at 1.6 V. The concentration in the depletion region left of the barrier depends on the injected current and is thus correlated to the concentration in the well.

Method G1 and Method G2 are equally well suited for this resonant tunneling structure. Method G3 and Method G4 can be used as well, however, in that case one has also to assess the error due to the small imbalance of positive and negative particles generated. Method I1 and Method I2 could not be used as they produce prohibitively large variance.

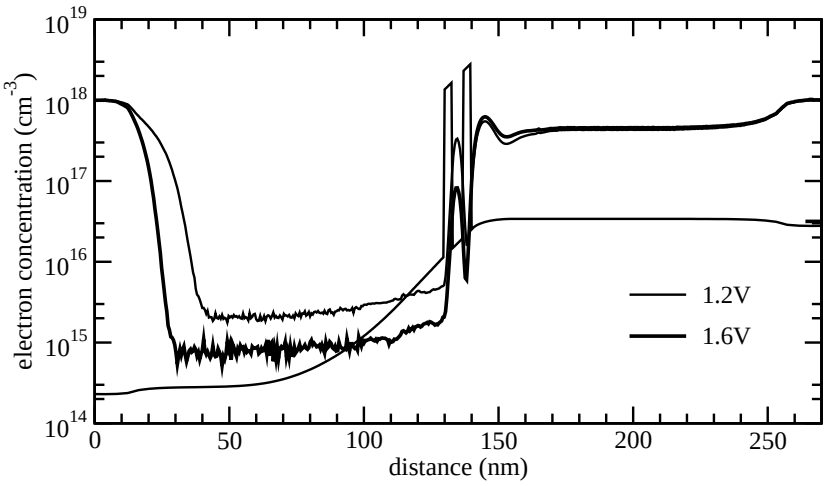

Figure 5: Electron concentration profiles in a resonant tunneling diode.

Conclusion

The position-dependent Wigner equation has been used to model nanoelectronic devices. The equation is transformed to an integral form and various forward estimators for the solution of this equation are discussed. Six estimators are described in terms of particle models, comprising transition probabilities and expressions for the particle weight. The fact that the kernel can assume negative values leads to instable particle models. Two of the presented models show exponentially increasing particle weights, and four models exponentially increasing particle numbers. The growth rate in all these models is given by the L_1 norm of the Wigner potential, termed $2\gamma = \int |V_w(\mathbf{q})| d\mathbf{q}$ in this work. A stable MC algorithm can be constructed by combining a particle generation model with a particle annihilation method.

References

[1] L. Shifren, D. Ferry, Wigner function quantum Monte Carlo, Physica B 314 (2002) 72–75.

[2] P. Bordone, A. Bertoni, R. Brunetti, C. Jacoboni, Monte Carlo simulation of quantum electron transport based on Wigner paths, Mathematics and Computers in Simulation 62 (2003) 307–314.

[3] M. Nedjalkov, R. Kosik, H. Kosina, S. Selberherr, Wigner transport through tunneling structures – scattering interpretation of the potential operator, in: Proc. Simulation of Semiconductor Processes and Devices, Business Center for Academic Societies Japan, Kobe, Japan, 2002, pp. 187–190.

[4] H. Kosina, M. Nedjalkov, S. Selberherr, Quantum Monte Carlo simulation of a resonant tunneling diode including phonon scattering, in: Nanotech, Computational Publications, San Francisco, 2003, pp. 190–193.

[5] M. Nedjalkov, H. Kosina, R. Kosik, S. Selberherr, A space dependent Wigner equation including phonon interaction, Journal of Computational Electronics 1 (1-2) (2002) 27–33.

[6] H. Kosina, M. Nedjalkov, S. Selberherr, Theory of the Monte Carlo method for semiconductor device simulation, IEEE Trans.Electron Devices 47 (10) (2000) 1898–1908.

[7] H. Kosina, M. Nedjalkov, S. Selberherr, The stationary Monte Carlo method for device simulation - part i: Theory, J.Appl.Phys. 93 (6) (2003) 3553–3563.

[8] H. Kosina, M. Nedjalkov, S. Selberherr, A Monte Carlo method seamlessly linking classical and quantum transport calculations, Journal of Computational Electronics 2 (2-4) (2004) in print.