Boundary Concepts for an Improvement of the Numerical Solution with regard to the Wigner Transport Equation

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***Abstract*—Even though the numerical solution of the Wigner Transport Equation is linked with problems, the approach is preferable from the engineering point of view. Among the several differences in comparisons based on the numerical solution of the Schrödinger equation, the absence of open boundary conditions may be one of the most prominent challenges. As a consequence unphysical results may be obtained. To overcome the limitations, two concepts are presented allowing an inclusion of open boundary conditions in the Wigner function formalism. The concepts are investigated by means of a simple structured resonant tunneling diode as a prototype device.**

***Index Terms*—Wigner Transport Equation, Computational Nanotechnology, open boundary conditions, self energy**

I. Introduction

With regard to highly performant engineered electronic devices sophisticated numerical methods are desirable. Along with the Wigner Transport Equation (WTE) quantum effects are inherently involved as well as scattering mechanisms can be implemented in detail. Unfortunately, conventional methods for the numerical solution of the WTE tend to have many problems. To start with, the diffusion operator is discretized utilizing an upwind difference scheme [1]. In particular, along with this approximation procedure the forward and backward traveling statistical distribution waves of the carriers are seperated from each other [2], although they should be coupled. As a consequence, coherent effects cannot be retained adequately leading to inherent errors. Additionally, conventional methods allow only the application of local boundary conditions, whereas nonlocal boundary conditions with respect to the nonlocal kinetic operator have to be considered [2], [3]. To overcome these limitations an approach based on the formulation of an exponential operator has been proposed recently [2]. Nevertheless, in this context the application of the exponential operator approach poses the question of the validity of the common Dirichlet boundary conditions with respect to the phase space coordinate k. Open boundary conditions, reflecting the nonlocal character of quantum mechanics, are needed.

To address this aspect, two feasible boundary concepts with respect to the k-coordinate applied to the WTE are discussed. Before this discussion starts, the fundamentals of the Wigner function formalism are briefly presented in section II for the sake of clarity. Then, in section III the boundary concepts are proposed and discussed. The validity of the concepts is demonstrated on the basis of a resonant tunneling diode in section IV. Finally, the contribution is closed by a summary and conclusion in section V.

II. Wigner Transport Equation

For a conventional one dimensional effective mass Hamiltonian the WTE is defined according to

$$\begin{aligned}\frac{\partial}{\partial t}f(\chi,k,t) = &-\frac{\hbar k}{m}\frac{\partial}{\partial \chi}f(\chi,k,t)\\ &-\frac{1}{\hbar}\int\frac{\mathrm{d}k'}{2\pi}\,V(\chi,k-k')f(\chi,k',t),\end{aligned} \tag{1}$$

where the variables χ, k and t represent the spatial, phase space and time dependency. Beyond, the constant $\hbar$ is the reduced planck's constant. For presentation purposes the effective mass distribution m is assumed to be spatially constant. The integral kernel $V(\chi, k-k')$ can be written as

$$\begin{aligned}V(\chi,k-k') = &\int \mathrm{d}\xi\ \sin\left((k-k')\,\xi\right)\\ &\times\left[v\left(\chi+\frac{1}{2}\xi\right)-v\left(\chi-\frac{1}{2}\xi\right)\right]\end{aligned} \tag{2}$$

with the function v being the potential distribution of the device. The potential v contains as well the conduction band distribution as the self-consistent Hartree-Fock-potential. Therefore, the term containing the potential is assigned to the drift effect, whereas the term containing the spatial derivative with respect to the χ-direction considers the diffusion effect.

In accordance with the concept of inflow and outflow boundary conditions, the Wigner function at the boundaries with respect to the spatial coordinate χ, located at χ_0 and χ_{N+1}, is given by the Fermi Dirac statistics $f_{\text{Fermi}}(k)$

$$\begin{aligned}f(\chi_0,k>0) &= f_{\text{Fermi}}(k>0)\\ f(\chi_{N+1},k<0) &= f_{\text{Fermi}}(k<0)\end{aligned} \tag{3}$$

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distinguishing between the sign of the values of the phase space variable k. It is well known, that the application of the Fermi Dirac statistic can be combined with problems [3]. Regarding the boundary conditions with respect to the k-direction, located at k_0 and k_{M+1}, conventional Dirichlet boundary conditions are assumed according to

$$\begin{aligned} f(\chi, k_0) &= 0 \\ f(\chi, k_{M+1}) &= 0 \end{aligned} \tag{4}$$

with the values symmetrically distributed around the origin according to $k_0 = -k_{M+1}$. Utilizing the exponential operator approach, coherent effects are retained so that the validity of the latter boundary condition has to be investigated. Due to the separated forward and backward traveling statistical distribution waves of the carriers, the boundary condition with respect to the phase space becomes less significant, when applying the upwind difference scheme.

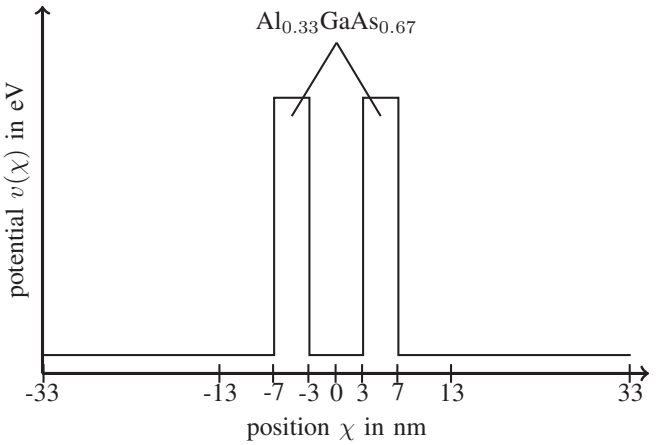


Fig. 1: Conduction band diagramm of the GaAs/$Al_{0.33}GaAs_{0.67}$ resonant tunneling diode.

III. Boundary Concepts

A. Transparent Boundary Condition

At first, following the concept of the self-energy terms, the exterior values of the Wigner function can be expressed dependent on the interior values of the Wigner function as stated by

$$\begin{aligned} f(\chi, k_0) &= a(\chi) \cdot f(\chi, k_1) \\ f(\chi, k_{M+1}) &= b(\chi)^{-1} \cdot f(\chi, k_M) \end{aligned} \tag{5}$$

where the functions $a(\chi)$ and $b(\chi)$ are the self-energy terms and, therefore, affect the open device behavior. Unfortunately, in comparison to the Schrödinger equation [4] and the nonequilibrium Green's function formalism [5], the self-energy terms $a(\chi)$ and $b(\chi)$ cannot be determined analytically.

Therefore, the inflow and outflow behavior with respect to the k-coordinate corresponding to the open boundary conditions has to be estimated from the interior values of the Wigner function, only. Following the idea of the estimation of the open boundary conditions, a standard technique could be applied, known as the transparent boundary condition scheme [6]. As this estimation has to be applied onto each discretized location, this approach is computational highly inefficient. Investigating this concept in practice, the estimation of the self-energy terms can suffer from the internal CPU accuracy.

B. Complex Absorbing Potential

Because of this fact, an alternative option is needed. So secondly, an external layer with respect to the k-coordinate can be introduced, which renders the open boundary conditions adequately leading to an appropriate description of the interior device physics. Until today, this concept is used for the numerical solution of the Schödinger equation [7]–[9] as for the numerical solution of electromagnetic wave propagation phenomena [10]. Especially, the latter concept, known as the perfectly matched layer technique, is the state of art technique. Therefore, the adaption of this concept is very promising for the application in the WTE. For this purpose, a complex absorbing potential $W(\xi)$ [7], [8] within the external layer is defined, leading to an artifcial damping of the Wigner function within the layer. As a consequence, the Wigner function represents a decaying function in the layer, enabling the application of the conventional Dirichlet boundary conditions. To avoid reflections from the external layer, which cause a nonphysical interference pattern within the Wigner function, the complex absorbing potential has to be matched to the interior interface.

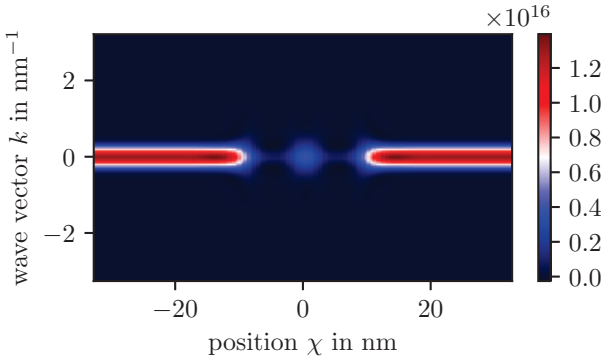
Due to this discussion, only the drift operator is affected by a further function introducing the complex absorbing potential. Investigating the symmetry properties of a general imaginary potential within the Wigner function formalism, an even symmetry can be easily identified. Because of this symmetry requirements, the function $W(\xi)$ has to be an even function with respect to the variable ξ. Furthermore, to fullfil the above conditions, the function $W(\xi)$ has to be chosen, such that its monotonously rising towards the boundary. At the interface of the internal device, the function $W(\xi)$ is zero valued. Therefore, for an inclusion in the conventional Wigner transport equation (1), the integral kernel in (2) is redefined according to

$$\begin{aligned} V(\chi, k-k') = \int d\xi \sin\left[(k-k')\xi\right] \\ \times \left[v\left(\chi + \frac{1}{2}\xi\right) - v\left(\chi - \frac{1}{2}\xi\right)\right] + \cos\left[(k-k')\xi\right] W(\xi). \end{aligned} \tag{6}$$

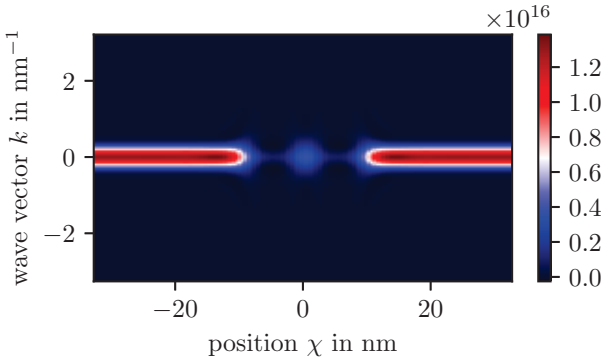
For the purpose of demonstration the function $W(\xi)$ is chosen to be

$$W(\xi) = \begin{cases} W_0 \cdot (\xi - \xi_0)^2 & \text{, if } \xi > \quad \xi_0 \\ W_0 \cdot (\xi + \xi_0)^2 & \text{, if } \xi < -\xi_0 \\ 0 & \text{, elsewhere} \end{cases}, \tag{7}$$

where the constant ξ_0 defines the location of the interface to the external layer. For all simulations, the parameters are set to be $\xi_0 = 20\text{nm}$ and $W_0 = 1/20\text{eVnm}^{-1}$, respectively. Note, that the property of the Wigner function being a real function

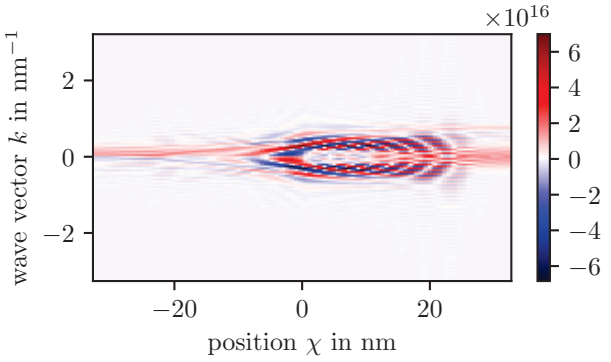


(a)

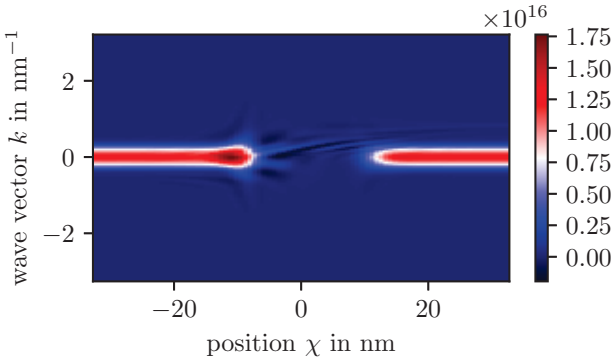


(b)

Fig. 2: Consideration of the thermal equilibrium Wigner functions. The Wigner function for the conventional boundary scheme is depicted in Fig. 2a, whereas the Wigner function for the proposed boundary scheme is shown in Fig. 2b.



(a)



(b)

Fig. 3: Nonequilibrium Wigner functions applying an external voltage of -0.33V. The conventional boundary scheme leads to the Wigner function depicted in Fig. 3a. In Fig. 3b the Wigner function for the case of the modified boundary scheme is depicted.

can be retained utilizing the concept of the complex absorbing potential.

IV. Numerical Examples

The advantages of the concept of the complex absorbing potential are demonstrated on a standard resonant tunneling diode based on the material system GaAs/$Al_{0.33}GaAs_{0.67}$ as depicted in Fig. 1 applying the exponential operator approach [2]. The quantum structure is based on the 6nm wide quantum well consisting of the material GaAs enclosed by the 4nm wide $Al_{0.33}GaAs_{0.67}$ barriers. All calculations are performed in relation to the bandgap energy of the material GaAs, leading to a maximum value of the potential of 0.261eV within the $Al_{0.33}GaAs_{0.67}$ barriers. The doping density in the contact regions is assumed to be 10^{18}cm^{-3}. Along with the ambient temperature of 300K, the chemical potential is given by 0.0462eV. The computational domain with respect to the χ-direction shows a length of 66nm and is discretized with 137 points, whereas the phase space in k-direction is discretized with 138 points.

For the sake of clarity, the results obtained for the case of the conventional Dirichlet boundary conditions are compared with the results additionally applying the external layer including the complex absorbing potential. In Fig. 2a the Wigner function for the case of the conventional Dirichlet boundary conditions and in Fig. 2b the Wigner function including the external layer is depicted, respectively. Both Wigner functions in Fig. 2a and Fig. 2b are calculated for the thermal equilibrium and show an excellent agreement. This agreement can be justified when considering the Wigner function as a correlation of different quantum states. The major correlations decay before they reach the boundary. Therefore, to identify the influence of the external layer, the resonant tunneling diode is investigated for the nonequilibrium case, applying an external bias of -0.33V. In this nonequilibrium state the correlations are not assumed to decay before the boundary of the computational domain is reached. The Wigner functions for the case of the nonequilibrium state are depicted in Fig. 3a applying the conventional Dirichlet boundary conditions and in Fig. 3b

with the additional external layer, respectively. Comparing the Wigner function in Fig. 3a and 3b, an unphysical interference pattern in the Wigner function shown in Fig. 3a can be observed. This unphysical pattern within the Wigner function is due to the inappropriate application of Dirichlet boundary conditions.

V. Summary and Conclusion

Two feasible concepts for an adequate inclusion of the open device behavior, reflecting the nonlocal behavior of quantum mechanics with respect to the phase space, have been presented. The implementation of the transparent boundary scheme is combined with numerical issues related to the internal CPU accuracy so that no physical results can be obtained from the methodology. The concept of the complex absorbing potential for an application in the field of the Wigner Transport Equation has successfully demonstrated by means of a simple structured resonant tunneling diode. Unphysical results as obtained from the conventional boundary scheme can be circumvented. In summary, the concept of the complex absorbing potential represents a substantial improvement for the numerical solution of the Wigner Transport Equation.

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References

[1] W. R. Frensley, "Quantum transport modeling of resonant tunneling devices," Solid-State Electron., vol. 31, no. 3/4, pp. 739 – 742, 1988.

[2] D. Schulz and A. Mahmood, "Approximation of a phase space operator for the numerical solution of the Wigner transport equation," J. Quantum Electron., vol. 52, no. 2, pp. 1–9, 2016.

[3] R. Rosati, F. Dolcini, C. Iotti and F. Rossi, "Wigner function formalism applied to semiconductor quantum devices: Failure of the conventional boundary condition scheme," Phys. Rev. B, vol. 88, pp. 3451–3466, 2013.

[4] C. S. Lent and D. J. Kirkner, "The quantum transmitting boundary method," J. Appl. Phys., vol. 67, no. 10, pp. 6353–6359, 1990.

[5] R. Lake and S. Datta, "Nonequilibrium Green's function method applied to double-barrier resonant-tunneling diodes," Phys. Rev. B, vol. 45, no. 12, pp. 6670-6685, 1992.

[6] G. R. Hadley, "Transparent Boundary Condition for the Beam Propagation Method,", J. Quantum Electron., vol. 28, no. 1, pp. 363-370, 1992.

[7] U. Riss and H. Meyer, "Calculation of resonance energies and widths using the complex absorbing potential method," J. Phys. B: At. Mol. Opt. Phys, vol. 26, no. 23, pp. 4503-4535, 1993.

[8] D. Neuhasuer and M. Baer, "The time-dependent Schrödinger equation: Application of absorbing boundary conditions," J. Chem. Phys., vol. 90, no. 8, pp. 4351-4355, 1989.

[9] A. Ahland, D. Schulz and E. Voges, "Accurate mesh truncation for Schrdinger equations by a perfectly matched layer absorber: Application to the calculation of optical spectra," Phys. Rev. B, vol. 60, no. 8, 1999.

[10] J. Berenger, "A perfectly matched layer for the absorption of electromagnetic waves," J. Comput. Phys., vol. 114, no. 2, pp. 185-200, 1994.