Deterministic Solution of the Discrete Wigner Equation

Johann Cervenka(✉), Paul Ellinghaus, and Mihail Nedjalkov

Institute for Microelectronics, TU Wien, Vienna, Austria
cervenka@iue.tuwien.ac.at

Abstract. The Wigner formalism provides a convenient formulation of quantum mechanics in the phase space. Deterministic solutions of the Wigner equation are especially needed for problems where phase space quantities vary over several orders of magnitude and thus can not be resolved by the existing stochastic approaches. However, finite difference schemes have been problematic due to the discretization of the diffusion term in this differential equation. A new approach, which uses an integral formulation of the Wigner equation that avoids the problematic differentiation, is shown here. The results of the deterministic method are compared and validated with solutions of the Schrödinger equation. Furthermore, certain numerical aspects pertaining to the demanded parallel implementation are discussed.

Keywords: Discrete Wigner equation · Integral formulation

1 Introduction

An accurate description of carrier transport in nanoelectronic devices necessitates quantum mechanics to be considered. The Wigner formalism presents a convenient formulation of quantum mechanics in the phase-space, thereby allowing many classical notions and concepts to be reused [3,4].

Basis for the following considerations is the Wigner equation

$$\frac{\partial f(x,k,t)}{\partial t} - \frac{\hbar k}{m^*}\,\frac{\partial f(x,k,t)}{\partial x} = \sum_m V_w(x,k-k')\; f(x,k',t), \tag{1}$$

which describes the evolution of the Wigner function $f(\mathbf{r},k,t)$, under the influence of the Wigner potential V_w. A detailed explanation to the aspects of the Wigner formalism can be found in [6] for instance. Deterministic solutions of the Wigner equation have huge memory requirements, which has hampered practical implementations in the past. Stochastic methods avoid this problem, albeit usually by trading memory requirements for computation time. A further difficulty with deterministic methods lies in the discretization of the diffusion term in the differential equation, due to the the highly oscillatory nature of Wigner functions in the phase-space. Indeed the commonly used higher-order schemes show very different output characteristics. However, the precision of the deterministic methods make them the only possible approach in cases where physical quantities vary over many orders of magnitude in the phase space.

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2 Solution Approach

The developed deterministic approach uses the integral formulation of the evolution Wigner equation. The integral form [5,7] is obtained by considering the characteristics of the Liouville operator on the left-hand-side of (1), which are the Newtonian trajectories $x(\cdot, t)$ initialized with x', k', t':

$$x(x', k', t', t) = x' + \frac{\hbar k'}{m^*}(t - t'). \tag{2}$$

This approach has already been used for development of stochastic solvers, which rely on the corresponding Neumann series of the integral equation [1].

Here, we develop an alternative procedure by first discretizing the variables of the equation by:

$$x = n\Delta x,\ n \in [0, N]; \quad k = m\Delta k,\ m \in [-M, M]; \quad t = l\Delta t,\ l \in [0, L]$$

The numerical task is to calculate the mean value f_Θ – the integral of the solution inside a particular domain indicated by Θ. The indicator function Θ is unity if the phase-space argument belongs to the domain and zero otherwise.

$$f_\Theta(\tau) = \int_0^\tau \mathrm{d}t \sum_n \sum_m f_i(n, m)\, e^{-\int_0^t \gamma(x_i(y))\mathrm{d}y}\, g_\Theta(x_i(t), m, t), \tag{3}$$

where τ is the evaluation time, f_i the initial condition, $x_i(t)$ is the trajectory, initialized by $(n\Delta x, m\Delta k, 0)$, and g_Θ is the so-called forward solution of the adjoint integral equation:

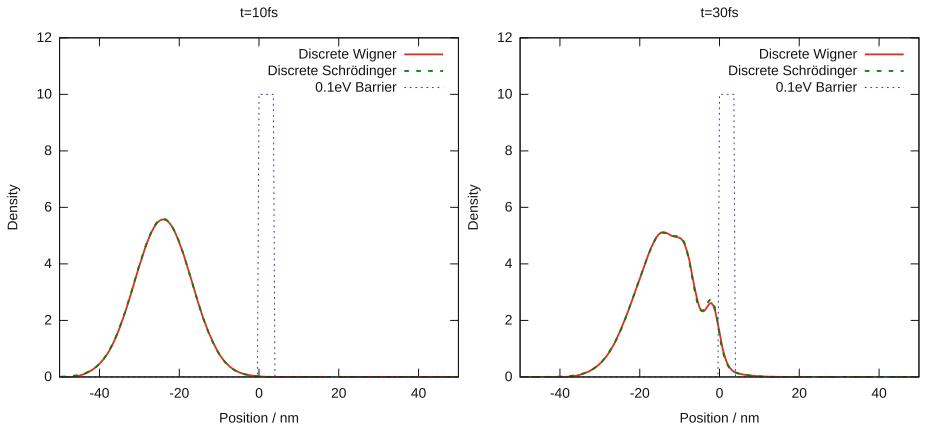

Fig. 1. Density after 10 fs and 30 fs for a wave package propagating through a 4 nm wide and 0.1 eV high potential barrier.

$$g_\Theta(n',m',t') = \Theta(n',m')\,\delta_{t',\tau} + \int_{t'}^{\tau} \mathrm{d}t \sum_m e^{-\int_{t'}^{t}\gamma(x(y))\mathrm{d}y}\,\Gamma(x(t),m,m')\,g_\Theta(x(t),m,t) \quad (4)$$

Within (4) $\gamma(n) = \sum_m V_w^+(n,m)$,

$$\Gamma(n,m,m') = V_w^+(n,m-m') + V_w^+(n,m'-m) + \gamma(n)\delta_{m,m'},$$

and $x(t)$ initialized by $(n'\Delta x, m\Delta k, t)$. All operations involving the time variable are also discretized. In particular, (2) may be expressed as

$$x(n',m,l',l) = \left(n' + int\left(\frac{\hbar m \Delta k \Delta t}{m^* \Delta x}(l-l')\right)\right)\Delta x. \quad (5)$$

For the moment we assume that the integral can be simply substituted by a summation and will return to the problem in the sequel.

3 Numerical Aspects of the Method

The value of f_Θ depends on the particular forward solution g_Θ and the initial condition f_i. The various values forming the initial condition evolve independently from each other in time and then are summated according to (3). Hence, to account for any arbitrary specified initial condition f_i, Eq. (4) must be solved for each domain $\Theta = \delta_{n',u}\delta_{m',v}$ associated to each point (u,v) of the region and evolution time $\tau = l_\tau \Delta t$. The simulation task entails solving

$$f_{u,v}(l_\tau) = \sum_{l=0}^{l_\tau} \Delta t \sum_n \sum_m f_i(n,m)\, e^{-\sum_{j=0}^{l}\gamma(x_i(j))\Delta y}\, g_{u,v,l_\tau}(x_i(l),m,l), \quad (6)$$

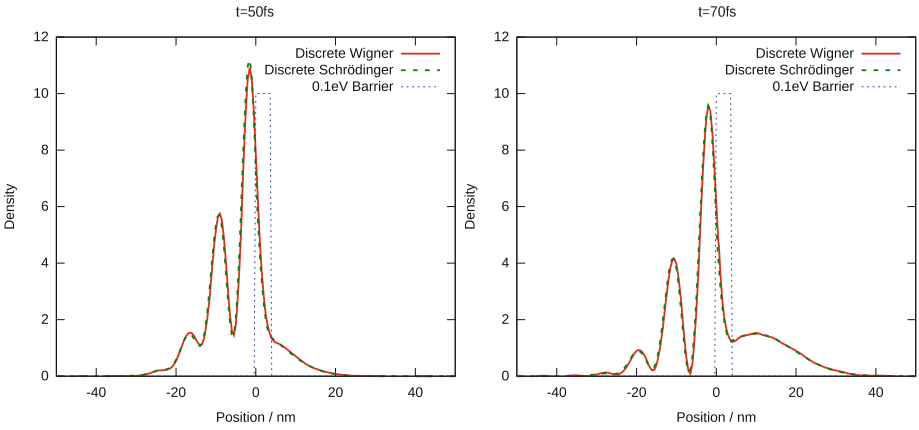

Fig. 2. Density after 50 fs and 70 fs for a wave package propagating through a 4 nm wide and 0.1 eV high potential barrier.

with

$$g_{u,v,l_\tau}(n',m',l') = \delta_{n',u}\delta_{m',v}\delta_{l',l_\tau} + \sum_{l=l'}^{l_\tau} \Delta t \sum_{m} e^{-\sum_{j=l'}^{l}\gamma(x(j))\Delta j}\,\Gamma(x(l),m,m')\,g_{u,v,l_\tau}(x(l),m,l). \quad (7)$$

For simplicity of the formulas we skip the initialization point in the notation of x and keep only the running variable.

Complexity of the Method

A direct implementation of the algorithm is to assemble and solve the equation system (4) of rank $L{\cdot}N{\cdot}2M$ (the number of spatial, momentum and time points) and then to back-insert the solution into (6).

This implies that the following algorithmic steps have to be repeated $L{\cdot}N{\cdot}2M$ times (for each particular indicator):

- assembly of (7) with effort $\mathcal{O}(2M \cdot L \cdot L)$,
- solving a system with rank $L \cdot N \cdot 2M$,
- back-insertion in (6) with effort $\mathcal{O}(L \cdot N \cdot 2M)$,
- the storage of all $g_\Theta(n', m', l')$
- the temporary storage for the equation system (7).

This analysis presents the upper bound for the estimated computational complexity. We suggest some optimizations to reduce the complexity in the following.

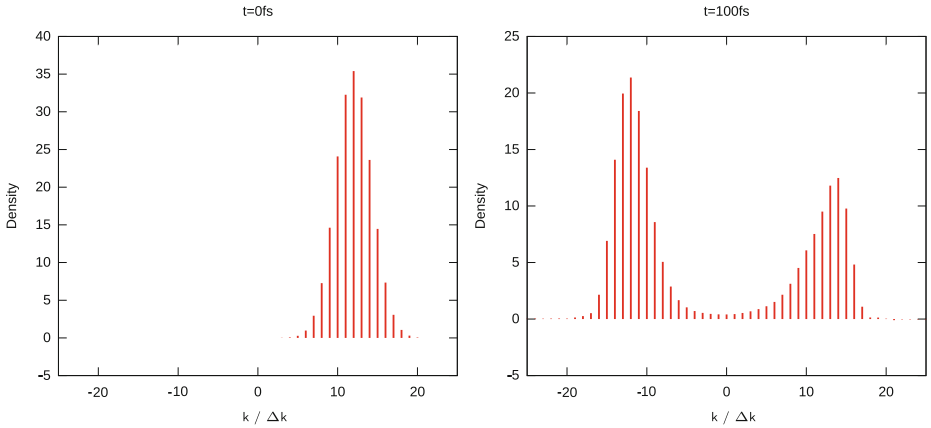

Fig. 3. The k-distribution at initial time and after 100 fs corresponding to Fig. 1. The transmission and reflection of the initially located wave around $k_0 = 12\Delta k$ can be seen.

Aspects of the Time Integration

An important improvement of the computation scheme is made by observing that the time-related quantity δ_{l',l_τ} may be accounted for analytically. Indeed, it may be shown that Eq. (7) becomes

$$g_{u,v,l_\tau}(n',m',l') = e^{-\sum_{j=l'}^{l_\tau}\gamma(x'(j))\Delta t}\delta_{x'(l_\tau),u}\delta_{m',v} + \sum_{l=l'}^{l_\tau}\Delta t \sum_{m} e^{-\sum_{j=l'}^{l}\gamma(x'(j))\,\Delta t\,\omega_j}\,\Gamma(x'(l),m,m')\,g_{u,v,l_\tau}(x'(l),m,l)\,\omega_l, \quad (8)$$

with $x'(l)$ initialized by n',m',l'. With this technique the time dependency in the back-insertion can be omitted and its complexity can be reduced. We note that Eq. (8) corresponds to a newly introduced higher-order integration scheme, since a detailed analysis has shown that higher-order discretization schemes have to be used. The used weights ω_l depend on the discretization of the integration.

Furthermore, examining the equation system (8) enables a recursion scheme where the already obtained forward solution is used to calculate the solution of the next time step. This allows a simplification in the rank of the equation system to $N \cdot 2M$.

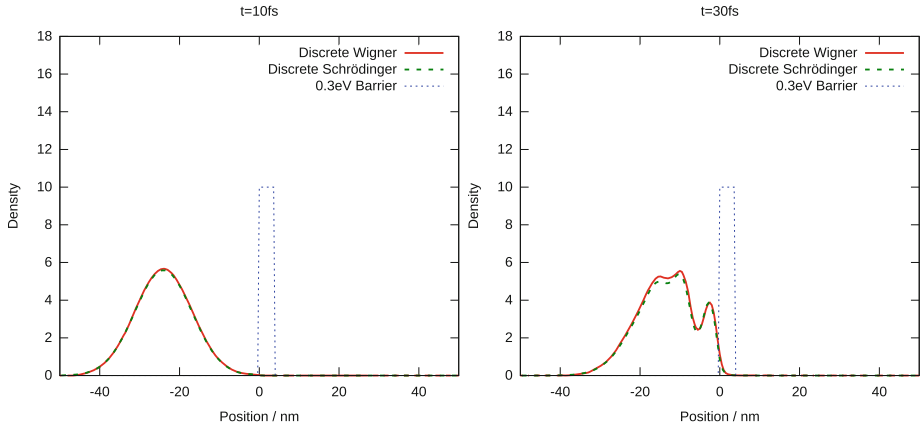

Fig. 4. Density after 10 fs and 30 fs for a wave package propagating through a 4 nm wide and 0.3 eV high potential barrier.

Computational Demands

The process step demanding the most computation time is the assembly of the equation system. The latter weights more heavily as evolution time increases, as the time steps to be summated and the summands in the exponent increase accordingly.

We further utilize the fact that the procedure, applied for each point (u,v,l_τ), depends only on the initial location in phase-space. Therefore, the calculation of

a certain point is independent on the processes associated with the rest of the points, making this method well-suited for parallelization as it proceeds without communications between the particular tasks. This enables an easy possibility of combining OpenMP on each node with Message Passing Interface (MPI) over several nodes. The communication overhead is only occasionally incurred when collecting the particular results $f_{u,v}(l_\tau)$ – this is reflected in the excellent scalability of the parallelization.

The increase of the evolution time brings a corresponding increase of the memory required to retain the history. Thus a serial implementation running on single node quickly reaches its memory limit, thereby limiting both the achievable resolution and simulated time for the simulation. Additionally, a parallel implementation has the advantage of splitting the memory demands between the particular nodes, thereby allowing acceptable time and phase-space resolution to be achieved.

4 Application to a Wave Packet

The time evolution of a wave packet, which captures both particle- and wave-like physical characteristics, is an effective tool to study quantum transport in nanoscale semiconductor devices [2].

As a benchmark problem a minimum uncertainty wave packet [3]

$$\Psi_i(x, t = 0) = e^{-\frac{(x-x_0)^2}{2\sigma^2}} e^{ik_0 x} \tag{9}$$

is chosen, traveling to the right towards a square potential barrier. To apply this setting to the Wigner equation, the distribution of the potential barrier $V(x)$ has to be transformed by

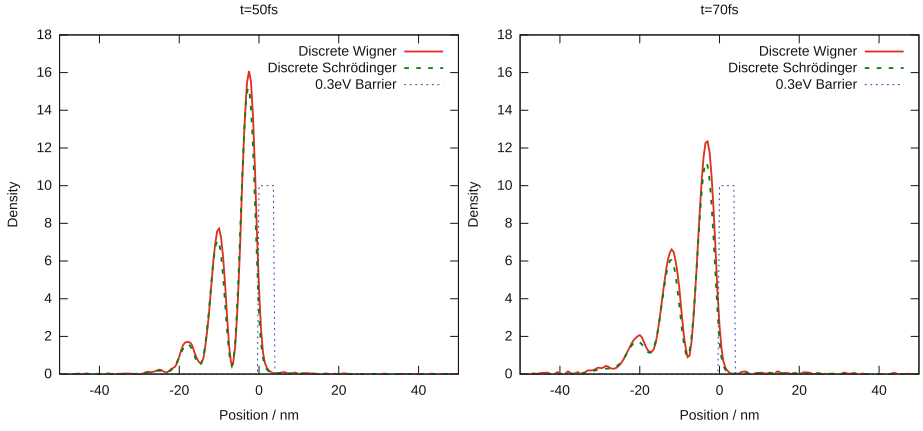

Fig. 5. Density after 50 fs and 70 fs for a wave package propagating through a 4 nm wide and 0.3 eV high potential barrier.

$$V_w(x,m) = \frac{1}{i\hbar}\frac{1}{L_{\mathrm{coh}}} \int_{-L_{\mathrm{coh}}/2}^{L_{\mathrm{coh}}/2} e^{-i2m\Delta k s} \left[V(x+s) - V(x-s)\right] \mathrm{d}s \tag{10}$$

to Wigner space. This formula is very general for the Wigner formalism, e.g. any wave function Ψ or any potential give their Wigner counterparts by such integral transform [6]. Here L_{coh} describes the desired coherence length of the system.

The parameters of the simulation are

- $x_0 = -29.5\,\mathrm{nm}$ the initial position of the peak of the wave packet,
- $\sigma = 10\,\mathrm{nm}$ the standard deviation in space of the initial wave package,
- $k_0 = 12\Delta k$ the speed of the wave packet,
- $\Delta k = \pi / L_{\mathrm{coh}}$ is the chosen spacing in phase-space, with
- $L_{\mathrm{coh}} = 100\,\mathrm{nm}$ the coherence length for the Wigner transformation.

To validate the results of the developed deterministic method, they are compared to the numerical solution of the one-dimensional Schrödinger equation [8]

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\Psi(x,t). \tag{11}$$

Figures 1 and 2 show the solutions of the Wigner equation, solved by the deterministic method, compared to the solution of the Schrödinger equation for a wave packet traveling through a 4 nm wide, 0.1 eV high barrier at various time steps. A good accordance between the results can be seen. The corresponding distribution in k-space can be seen in Fig. 3. Here, the transmitted and reflected parts of the wave can be clearly observed. The simulations were performed using a 200×50 grid in the phase-space, with a spatial resolution of $\Delta x = 0.5\,\mathrm{nm}$

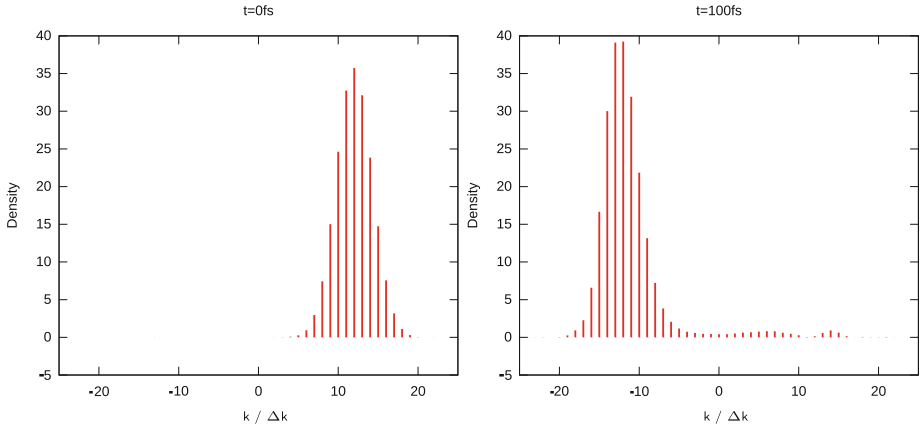

Fig. 6. The k-distribution at initial time and after 100 fs corresponding to Fig. 4. The nearly total reflection of the initially located wave around $k_0 = 12\Delta k$ can be seen.

and $\Delta k = \pi/100\,\text{nm}$. The time discretization used a step-with of $\Delta t = 0.5\,\text{fs}$ to maintain a good accuracy for the transmitted part of the wave packet.

Figures 4 and 5 show the same initial wave approaching a 0.3 eV high barrier. Here, the wave is almost completely reflected. The corresponding k-distribution can be seen in Fig. 6 for 0 fs and 100 fs, which shows nearly the same shape as the former but reversed sign in k-space. Both examples show an excellent accordance between the numerical solution of the Schödinger equation – the mainstay for quantum transport simulations – and the deterministic solution of the Wigner equation.

5 Conclusion and Outlook

A novel method for deterministically solving the Wigner equation has been shown and validated by a comparison with the Schrödinger equation. Several improvements of the history calculation and interpolation schemes seem feasible and offer the most potential for speed-up. In the future the method will be applied to scattering processes and may be useful as pre-conditioner for stochastic Wigner methods.

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