# Spectral force approach to solve the time-dependent Wigner-Liouville equation

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The Wigner-Liouville (WL) equation is well suited to describe electronic transport in semiconductor devices. In the effective mass approximation the one dimensional WL equation reads

$$\frac{\partial}{\partial t}f(x,p,t)+\frac{p}{m}\frac{\partial}{\partial x}f(x,p,t) - \frac{1}{\hbar^2}\int \mathrm{d}p'\, W(x,p-p')f(x,p',t)=0, \quad (1)$$

with the Wigner kernel given by

$$W(x,p)=-\frac{\mathrm{i}}{2\pi}\int \mathrm{d}x' \exp\left(-\mathrm{i}\frac{px'}{\hbar}\right) \left[V\left(x+x'/2\right)-V\left(x-x'/2\right)\right]. \quad (2)$$

The Wigner kernel introduces a non-local interaction with the potential $V(x)$, in accordance with quantum theory. Unfortunately, even for this simple interaction the mathematical form includes a highly oscillatory component ($\exp\left[-\mathrm{i}\frac{\mathbf{p}\cdot\mathbf{x}}{\hbar}\right]$) which impedes stable numerical implementation based on finite differences or finite elements.

## Leveraging the Force

Using the force $F(x)=-\mathrm{d}V(x)/\mathrm{d}x$ instead of the potential yields a new expression of the Wigner kernel. By further expanding the force in terms of its Fourier components $F(x)=\int \mathrm{d}k\tilde{F}(k)e^{\mathrm{i}kx}$ a factor $k^{-1}$ emerges as seen in (3). This factor provides a natural damping of the highly oscillatory components of the Wigner kernel. Furthermore, this process yields a much simpler WL equation, local in $x$ and containing only a single integral over momentum,

$$\frac{\partial}{\partial t}f(x,p,t)+\frac{p}{m}\frac{\partial}{\partial x}f(x,p,t)-\int \mathrm{d}k\,\frac{\tilde{F}(k)e^{\mathrm{i}kx}}{\hbar k} \left[f\left(x,p-\frac{\hbar k}{2},t\right)-f\left(x,p+\frac{\hbar k}{2},t\right)\right]=0. \quad (3)$$

In the classical limit, for momenta $p>>\hbar k$ the Boltzmann equation emerges naturally.

## Quantum Generation

The new form of WL equation (3) can be interpreted as Newtonian transport of free particles [1], [2] (first two terms of the LHS), and a "quantum generation" term that mediates the force (last term of the LHS). The generation term is responsible for the production of symmetric positive and negative contribution at momenta $p+\hbar k/2$ and $p-\hbar k/2$ with a rate $\tilde{F}(k)e^{\mathrm{i}kx}/(\hbar k)f(x,p,t)$. As such it is closely related to the Wigner Monte-Carlo approach by Sellier et al.[3] The rate is directly proportional to the spectral component of the force at $k$. Higher frequency components of the force represent the quantum corrections with respect to the Boltzmann picture.

## Implementation

We implemented (3) based on a discretized position $x_i$, and momentum $p_j$. The momenta $p_j=\hbar k_j$ naturally follow from the FFT of the force $F[x_j]$ to $\tilde{F}[k_j]$, replacing the integral over $k$ with a finite sum over $k_j$. An initial condition $f_0[x_i,p_j]$ is chosen and the system is solved by stepping through time until a steady state is reached.

As a proof-of-concept we simulated an electron flow through a periodic potential as seen in figure 1. For the sake of clarity, and to aid comparison with the Landauer formalism, no net force has been applied. Electrons are injected from the left-contact with a Fermi-Dirac distribution ($E_\mathrm{F}=2\mathrm{eV}, T=0\mathrm{K}$), while no electrons are injected from the right side. The time evolution can be followed in figures 3, 4 and 5. We observe quantum effects such as transmission through mini-bands, as well as reflection at energies exceeding the barrier height. Comparison with a finite elements solver for the single electron Schrödinger equation coupled with ballistic Landauer transport is presented in figure 2.

## References

[1] M. Nedjalkov et al., *Unified particle approach to Wigner-Boltzmann transport in small semiconductor devices*, Phys. Rev. B **70**, 115319 (2004).
[2] D. Sels et al., *Classical trajectories: A powerful tool for solving tunneling problems*, Physica A **391**, 78-81 (2012).
[3] J.M. Sellier et al., *Two-dimensional Transient Wigner Particle Model*, SISPAD **18**, 404 (2013).

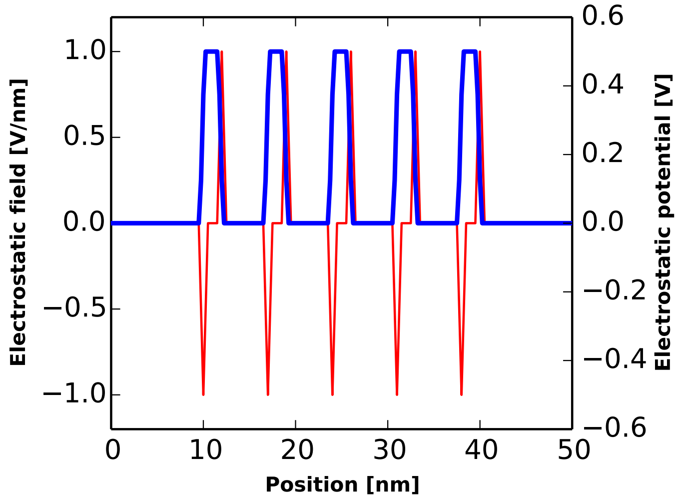



Fig. 1. The electrostatic potential *[bold/blue]* and field *[thin/red]* of the periodic potential

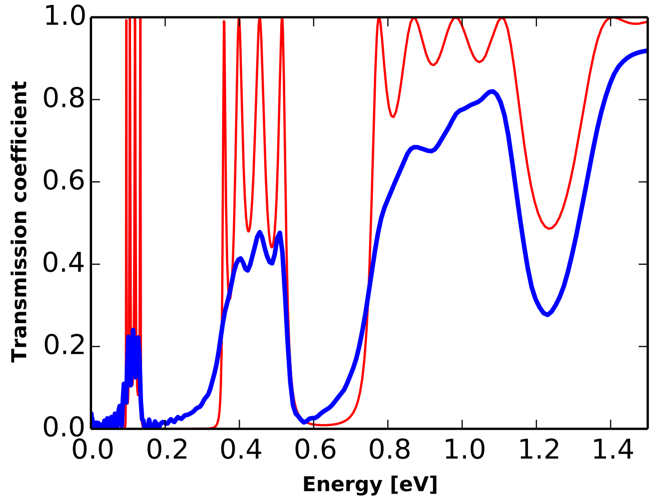
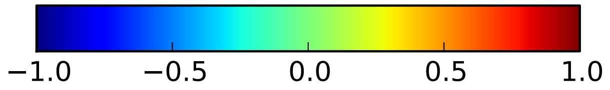



Fig. 2. Comparison of the transmission between the steady state solution of the time-evolved Wigner-Liouville *[bold/blue]* equation in the right contact, and the time-independent single electron Schrödinger/Landauer *[thin/red]* approach. Note we have good qualitative agreement as transmission occurs through the same subbands. The differences in absolute value are expected and subjected to further study, they are probably related to diffusion current which is not considered in the Schrödinger/Landauer approach.



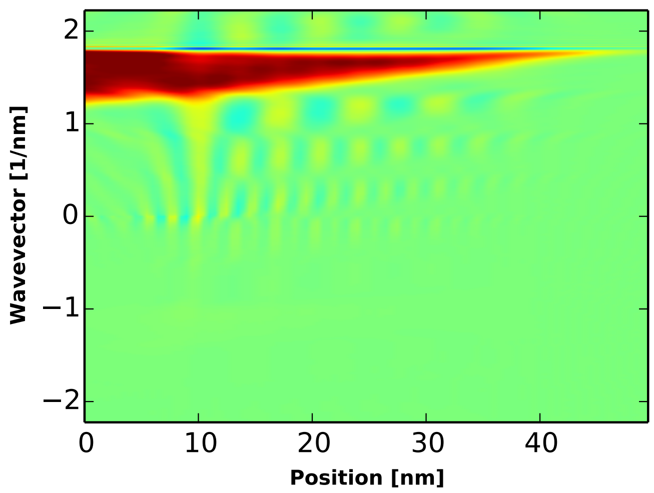



Fig. 3. The Wigner function after 43.3fs.

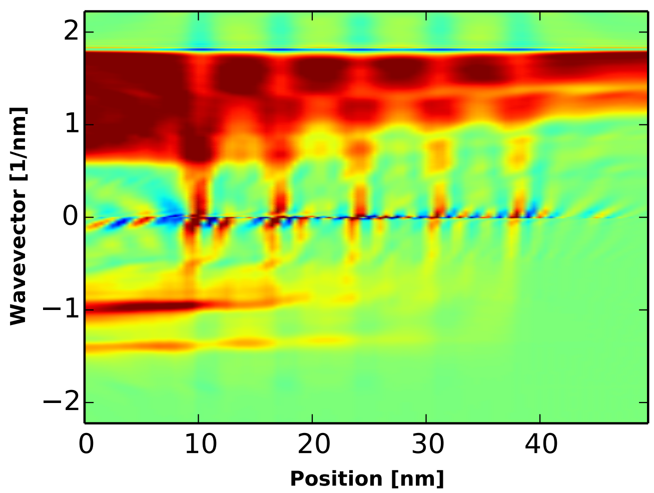



Fig. 4. The Wigner function after 86.6fs.

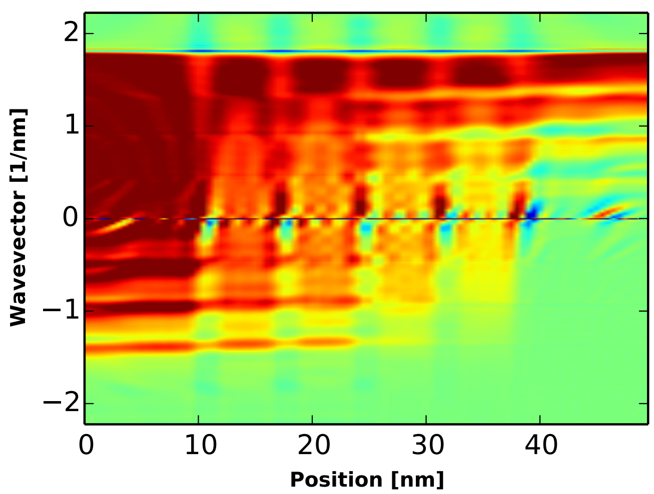



Fig. 5. The Wigner function in steady state, after 5ps.