# Semi-Discrete 2D Wigner-Particle Approach

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## SEMI-DISCRETE FORMULATION

The Wigner function (WF) approach to device simulations is regarded as convenient, as it maintains many classical concepts describing evolution and dissipation processes, as well as discouraging, due to many open numerical and theoretical issues: The approach has been applied to merely 1D problems, an increase of the dimensions has been considered impossible for computational reasons. Recent theoretical studies [1] show that the conventional WF formulation conflicts with the open system boundary conditions giving rise to unphysical effects. The problem is avoided if (i) the plane wave basis of the infinite Weyl-Wigner transform is replaced by a generic basis set [1]; (ii) the coherence integral of the transform is bounded inside the device by the assumption of vanishing correlation with the states in the leads [2]. Otherwise the coherence length becomes a free numerical parameter, which affects the computed physical quantities.

We propose an approach for 2D WF simulations, which fixes the above ambiguities and gives rise to a semi-discrete formulation of the Wigner equation. In particular the geometry of the conventional device in Fig. 1 leads to coherence integrals bounded into a rectangle along $x$ and $y$. In the spirit of (i) this allows to use the discrete Fourier basis corresponding to the rectangle. The obtained WF $f_w(\mathbf{r}, \mathbf{m}\Delta\mathbf{p})$ is continuous with respect to the position and discrete with respect to momentum, where $\mathbf{m} = (m_x, m_y)$ and $m_{x,y}$ are integers. The equation retains its usual form, but the momentum integral is replaced by an infinite sum, which simplifies the numerical treatment.

## NUMERICAL ASPECTS

The numerical treatment is difficult, but feasible in the framework of the developed Monte Carlo (MC) method. It utilizes the particle generation-annihilation algorithm [3], implemented on top of a standard 2D MC simulator as follows: Particles evolving in the classical way and equipped by a sign, which carries the quantum information, interact with the Wigner potential $V_w$. An interacting particle gives rise to two novel particles, generated locally in $\mathbf{r}$ but having different momentum and sign. Between the evolution steps particles are stored in a mesh defined in the phase space. Two particles with opposite sign annihilate in a given mesh cell. The presented scheme explores the convergence of the coherent task. First standard simulations provide the self-consistent potential in the device, Fig. 2. The potential gives the driving force, which forms the classical density in Fig. 3. Next the entire potential is used to obtain $V_w$. The driving force is zero, particles perform a free motion. In this case generation-annihilation processes form the quantum density shown in Fig. 4 and analyzed in the caption. The obtained averages for the density and other quantities are qualitative and mainly prove the convergence of the method. Many issues like dependence on the numerical parameters, the existence of alternative algorithms for boundary injection and normalization must be explored by a comparison with an independent quantum simulator. This procedure is currently underway. Interaction with phonons will be included on a next stage, which, however is straightforward for the method.

## ACKNOWLEDGMENT

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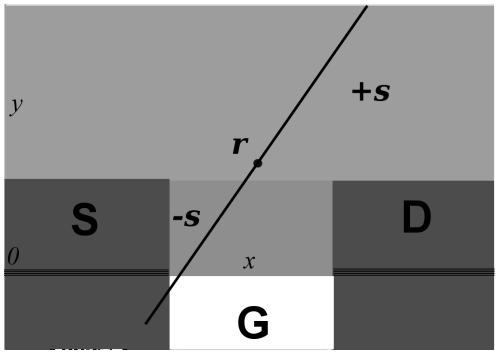


Fig. 1. A conventional 2D device structure: The Wigner function at given position $\mathbf{r}$ accounts for correlations in states between points symmetrically placed with respect to $\mathbf{r}$. The correlation becomes zero if one of the points belongs to a region with zero carrier density. It is due to the fact that the density matrix $\rho(\mathbf{r}+\mathbf{s}, \mathbf{r}-\mathbf{s})$ vanishes if one of the coordinates is outside the device boundaries $(0, L_x; 0, L_y)$. This is the case of no correlation with the states in the leads. If the correlation is not vanishing, the segment in $G$ is excluded along with the corresponding counterpart in the device. Then the integrals vanish outside the rectangle $(0, L_x; -L_y, L_y)$.

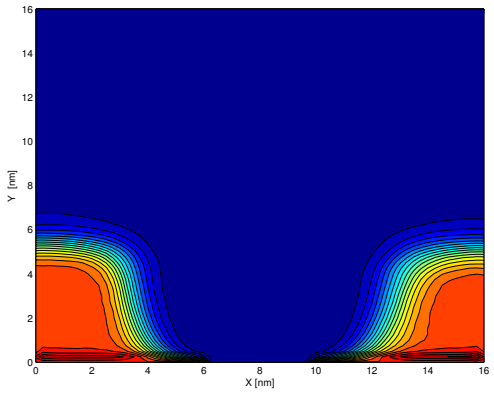


Fig. 3. Surface plot of the classical density: The carriers injected into the S/D regions from the $y = 0$ boundary are entirely separated by the high barrier and the potential in the substrate.

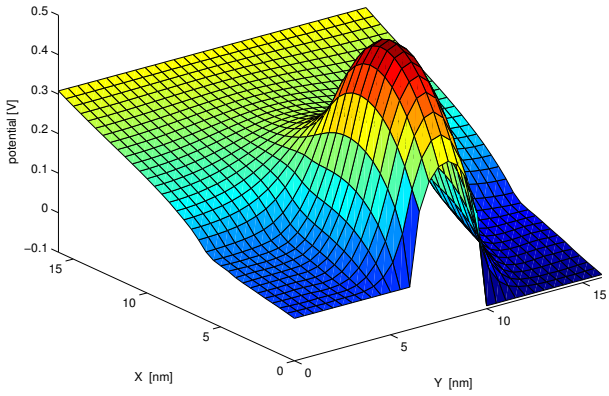


Fig. 2. Potential profile in a $16 \times 16nm$ device. The S/D regions are of $6nm$ width and depth, the substrate is $10nm$. The $4nm$ thick and $6nm$ long barrier rapidly drops on both sides of the $0.45V$ peak and demonstrates strong asymmetry in both directions. It is the central entity, selected to govern the quantum effects into a particular pattern. For this reason a rather peculiar doping concentrations have been chosen, holes are excluded from the simulations, and, as already noted, phonons are switched off.

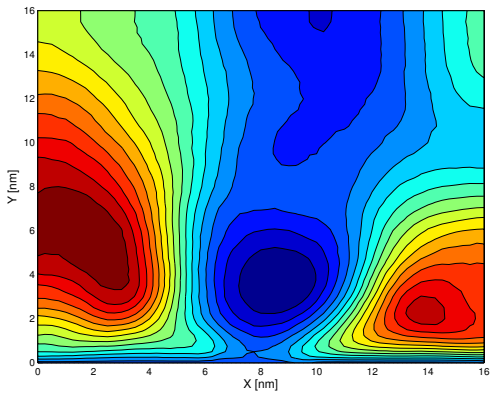


Fig. 4. Surface plot of the density obtained from the Wigner function. A comparison with the classical density outlines effects of tunneling and separation. The plot follows the pattern imposed by the potential. In particular, the region below the barrier peak is well pronounced by the lack of carriers; however an increase of the density is seen on both sides of the peak. The density is calculated on a regular, $0.25nm$ mesh. The corresponding Wigner function is comprised of more than $16 \times 10^6$ phase space elements. This precludes the application of the standard deterministic methods. The utilized Monte Carlo method maintains the number of positive or negative particles in each cell which is of a short integer datatype.