Electron Evolution and Boundary Conditions in the Wigner Signed-Particle Approach

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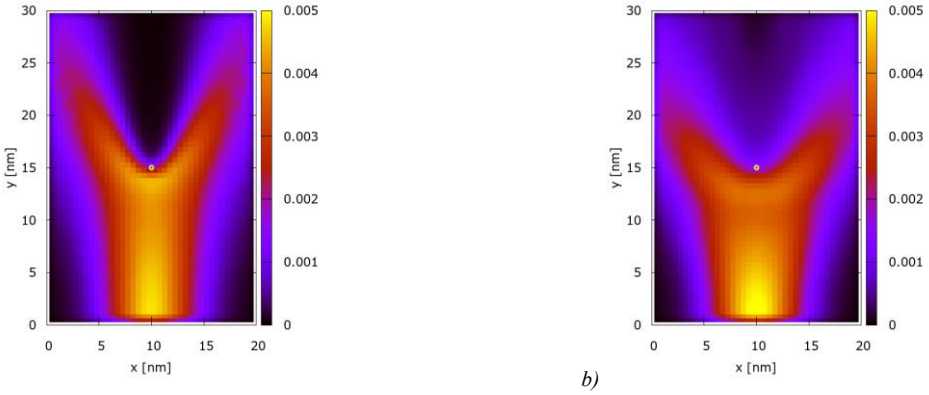
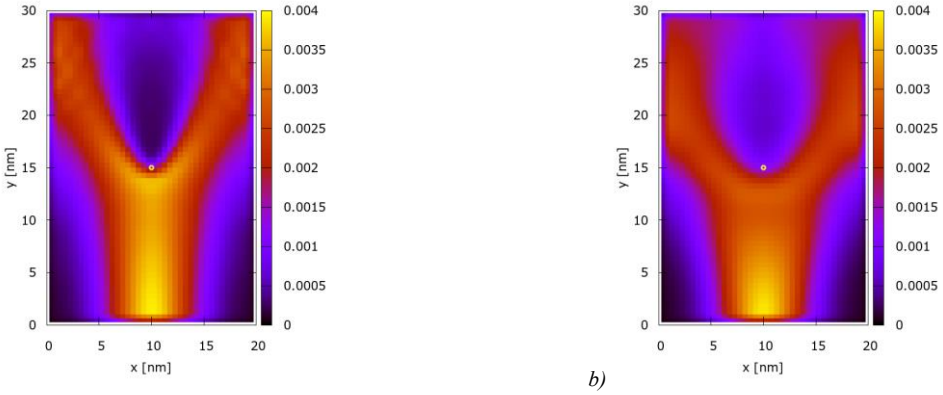
In modern nanoelectronics understanding quantum current transport is a fundamental challenge. In turn, in quantum mechanics evolution is driven by all the derivatives of the electric potential so rapid spatial variations of the potential can determine non-local effects, tunneling, and also interference phenomena. Those effects give rise to a complex interplay and cannot be decomposed in elementary processes to analyze separately. Thus, numerical modeling is a fundamental tool for studying quantum phenomena, since it allows to consider specific conditions that are difficult to implement by experimental approaches, e.g., switching between different boundary conditions to see how this affects the electron evolution [1] or de-activating scattering events [2]. The Wigner formulation of quantum mechanics provides a seamless transition to classical evolution, that represents a reference to highlight quantum effects [3]. In the signed-particle approach [4], electron evolution is modeled by the evolution of numerical particles that move along Newtonian trajectories and carry a sign. This aspect simplifies the implementation of "classical" boundary conditions, generally unfeasible in practice experimental approaches. We analyze the electron evolution against a repulsive dopant with a maximum potential energy of 0.175 eV with two different lateral boundary conditions [5]: absorbing boundaries, Fig. 1, and perfect reflecting boundaries, Fig. 2. From the comparison between the quantum electron density, Fig. 1b), and corresponding classical counterpart, Fig. 1a), we can notice the non-locality effects before and around the dopant, and also the tunneling that increased the quantum electron density in front of the dopant. Fig. 3a) shows the ratio between quantum and classical electron density, allowing to witness both the decrease below unity due to nonlocal effects and the peak in front of the dopant that reaches the maximum of 14 due to tunneling effects. In Fig. 2a) and Fig. 2b), we show the same scenario but for lateral reflecting boundaries. The electrons reflected from the lateral boundaries, both in the quantum and in the classic case, are injected in front of the dopant but in the quantum case the electron density is much more closed around the dopant due to the interplay of the non-locality and tunneling effects. As shown in Fig. 3b), the quantum density continues to be greater than the classic one in front of the dopant but now limited to a factor of 3 since the electrons reflected by the boundaries mitigate the effect of tunneling.



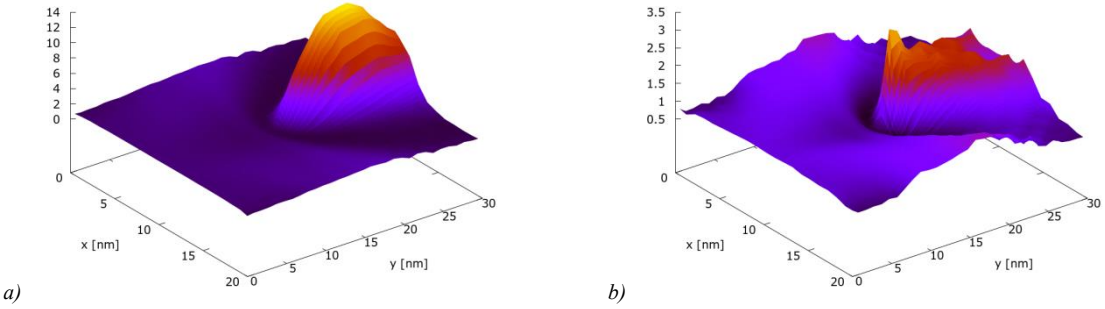
a) b)

Fig. 1: Electron density around the dopant with 0.175 eV peak energy (yellow isoline represents the 0.15 eV level) with lateral absorbing boundary condition: a) classical evolution, b) quantum evolution.



a) b)

Fig. 2: Electron density around a dopant with 0.175 eV peak energy (yellow isoline represents the 0.15 eV level) with lateral reflecting boundaries: a) classical evolution b) quantum evolution.



a) b)

Fig. 3: Ratio between quantum and classical electron density: a) lateral absorbing boundaries, b) lateral reflecting boundaries.

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