

## Classical and Quantum Electron Evolution with a Repulsive Dopant

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Modeling gives a unique opportunity to study quantum effects governing nanoelectronics by comparing them to classical effects and by selectively investigating different physical conditions which characterize the transport picture. To that end, the Wigner transport model implemented by a signed particle approach [1] can be reduced to the Boltzmann transport model, when the quantum rules for particle evolution are replaced by classical ones. The role of physical conditions can then be investigated in detail, such as using classical or quantum boundary conditions in order to enable or disable the effects of quantum repulsion [2]. In this work, we investigate the classical and quantum electron evolution with a repulsive dopant potential with ViennaWD [3]. In the classical case the evolution is local (the first derivative of the potential). However, in the quantum case all derivatives of the potential control the evolution. This gives rise to non-local and tunneling effects which both can be conveniently studied by means of simulation. In our particular simulation setup, the dopant potential is placed in the center of the simulation domain ( $20 \times 30 \text{ nm}^2$ ) and has a peak energy of about  $0.345 \text{ eV}$ . We inject a minimum uncertainty Wigner state [4] every  $1 \text{ fs}$  with an initial kinetic energy of  $0.141 \text{ eV}$ . Fig. 1 and Fig. 2 show the electron density for all absorbing boundary conditions in the classical and in the quantum case, respectively. The green *isoline* shown in all figures is the potential energy of the dopant at  $0.175 \text{ eV}$ . The non-locality effects of the quantum potential affect the injected electrons right after injection. Tunneling effects are identified due to the intensified spreading of the density. In Fig. 3 and Fig. 4 the current density is shown for  $10 \leq y \leq 30 \text{ nm}$ . The increasing quantum current density above the center is due to the action of the repulsive potential on the tunneling electrons. Adding classical reflecting boundaries on the lateral sides ( $x = 0$  and  $x = 20 \text{ nm}$ ) allows to cleanly study the effects of non-locality and tunneling without imposing effects of quantum repulsion. Fig. 5 and Fig. 6 show the current density with lateral reflecting boundaries. In this case the current's evolution path is much more closed around the dopant in the quantum case. This is attributed to the joint effect of tunneling and repulsion, since the electrons reflected from the boundary are accelerated after the dopant.

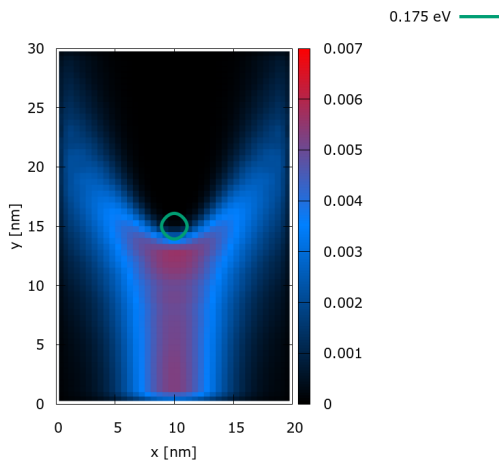


Fig. 1: Classical electron density [a.u.]; absorbing boundaries.

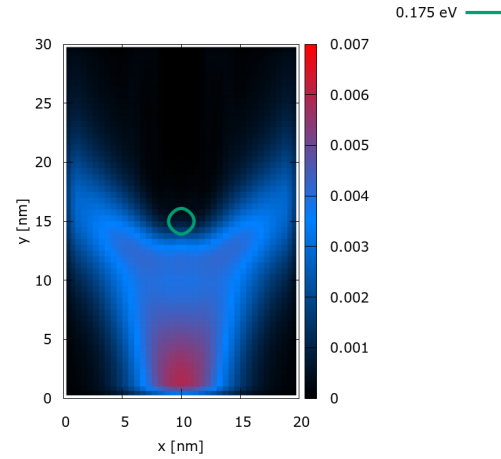


Fig. 2: Quantum electron density [a.u.]; absorbing boundaries.

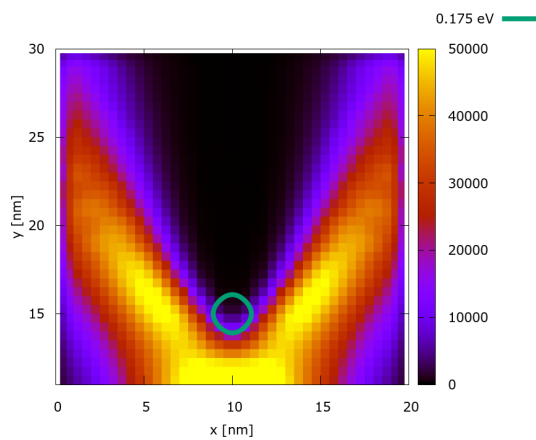


Fig. 3: Classical current density [a.u.]; absorbing boundaries (zoom).

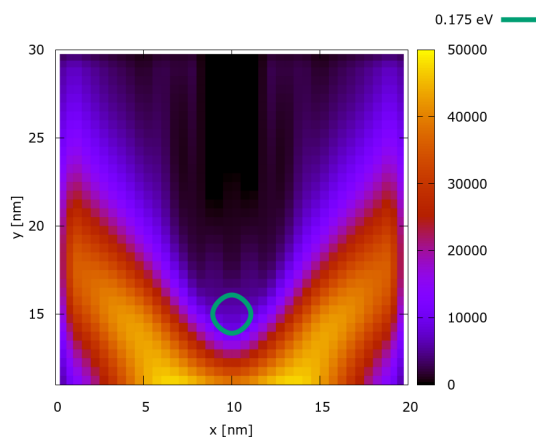


Fig. 4: Quantum current density [a.u.]; absorbing boundaries (zoom).

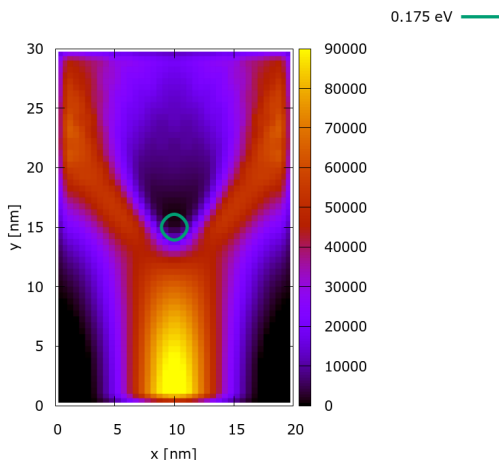


Fig. 5: Classical current density [a.u.]; lateral reflecting boundaries.

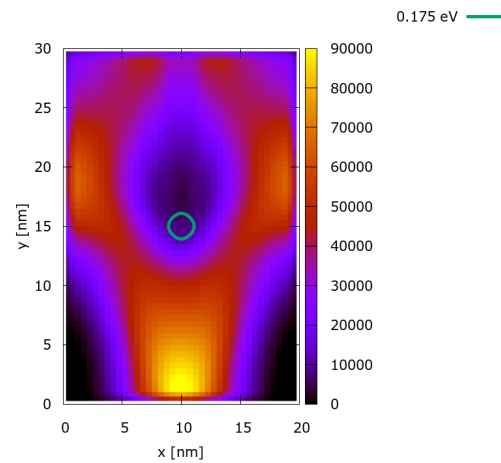


Fig. 6: Quantum current density [a.u.]; lateral reflecting boundaries.

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