

Wigner-Signed Particles Study of Double Dopant Quantum Effects

Josef Weinbub¹, Mihail Nedjalkov², Ivan Dimov³, and Siegfried Selberherr²

¹Christian Doppler Laboratory for High Performance TCAD at the

²Institute for Microelectronics, TU Wien, Austria

³IICT, Bulgarian Academy of Sciences, Bulgaria

Josef.Weinbub@TUWien.ac.at

We investigate the quantum effects induced by two dopants positioned on the electron path in a structure which resembles a two-dimensional quantum wire. We use the signed particle model for analysis, which presents an alternative heuristic formulation of the Wigner transport picture [1]. The major attributes of the model are that point-like particles with classical features, such as drift over Newtonian (field-less) trajectories, carry the quantum information by their positive or negative sign which contributes to the physical averages $\langle A \rangle$, which, apart from the sign, can then be calculated as in the classical case. The Wigner potential determines a spatial probability map, according to which any particle generates two novel counterparts with a positive and negative sign, while the attributes of the initial particle remains unaffected [2]. Contrary to Boltzmann particles, which resemble electrons, signed particles bear a mere numerical character. In particular, the electron density in a given phase space unit cell is approximated by the difference of positive and negative particles. With the double dopant experiment we analyze the effect on the electron density by continuously injecting identical, minimum uncertainty Wigner states $f_w = N \exp\{-(r - r_0)^2/2\sigma^2\} \exp\{-(k - k_0)^2/2\sigma^2\}$ [3], aiming to maintain coherent conditions. Since any injected state may be interpreted as a classical distribution, we can conveniently use the Boltzmann picture as a reference frame: Classical particles move on un-accelerated Newtonian trajectories until closing in on the dopants, where they begin to feel the electric force (cf. green area in Fig. 1). After leaving the region the free movement continues until leaving the domain. The particle transport is mainly along the y-direction (from bottom to top), the correlation between the two symmetric left and right subdomains (i.e. $0 \leq x \leq 10nm$ and $10nm \leq x \leq 20nm$) happens merely between the dopants and the drain (i.e. $y = y_{max}$). We use quantum simulations, powered by *ViennaWD* [4], to provide a density distribution as shown in Fig. 2. In particular, r_0 is centered in the source contact ($x = 10nm$) of the wire and $\sigma_{x,y} = 2nm$, corresponding to the equilibrium distribution around k_0 with the effective mass $m^* = 0.19$ at $T = 300 K$, with a total simulation time of $400 fs$ and an injection period of $8 fs$; steady state is reached after about $200 fs$. To study processes giving rise to coherence, we perturb the correlation between the two subdomains by introducing an artificial *kill zone* along the vertical symmetry line within the area $9.5nm \leq x \leq 10.5nm$ and $22nm \leq y \leq 25nm$, where negative particles are eliminated. Such a perturbation does not affect the classical picture since, as discussed, there is no correlation between the subdomains separated by the kill zone, there are no negative particles. Furthermore, if the action of the Wigner potential, which ensures the coherence, is weak, the effect of such a kill zone can only increase the electron density. Fig. 3 shows the effect of the kill zone on the density distribution (compare to Fig. 2). For a more detailed analysis, Fig. 4 shows a comparison of the density along $y = 29 nm$: For the kill zone case (red dashed line) the results show the opposite effect as described above - a reduction of the density. This demonstrates the active role of the Wigner potential in the domain around the kill zone. The main conclusion is, that, in contrast to the classical case, there exists an active particle exchange (i.e. correlation) in the horizontal x-direction, which is of crucial importance for the system to maintain coherence.

1. J.M. Sellier et al., Phys. Rep. **577**, DOI: 10.1016/j.physrep.2015.03.001(2015).
2. M. Nedjalkov et al., Appl. Phys. Lett. **102**, DOI: 10.1063/1.4802931 (2013).
3. D. Querlioz and P. Dollfus, Wiley-ISTE, DOI: 10.1002/9781118618479 (2010).
4. ViennaWD, <http://viennawd.sourceforge.net/>

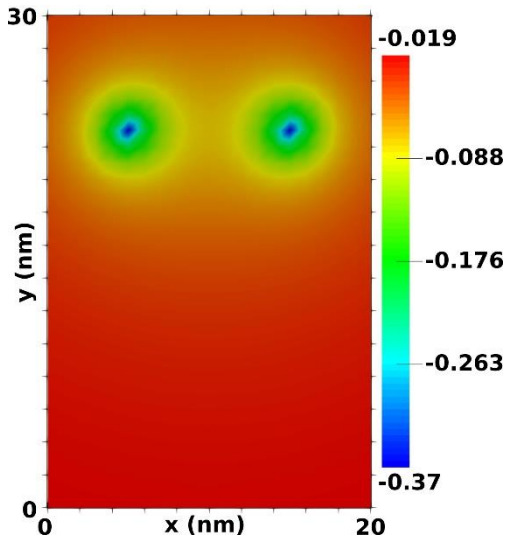


Fig. 1: Potential distribution in eV . The green region outlines the potentials of the two dopants. The setup is such that we can ignore a joint action of the corresponding forces.

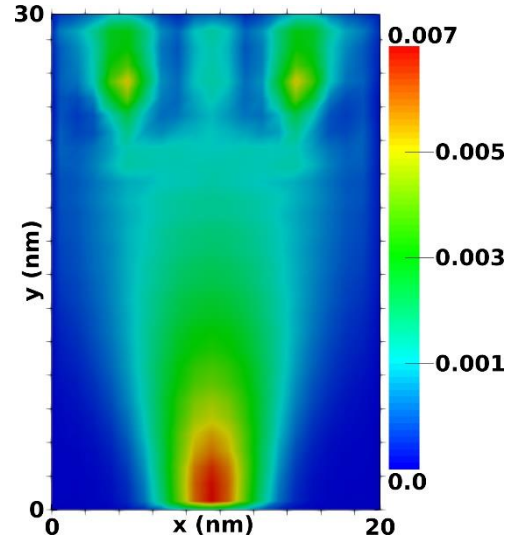


Fig. 2: After 200 fs quantum evolution the density (arbitrary unit) approaches a stationary distribution. No artificial borders are introduced; particles leaving the simulation domain in any direction are eliminated.

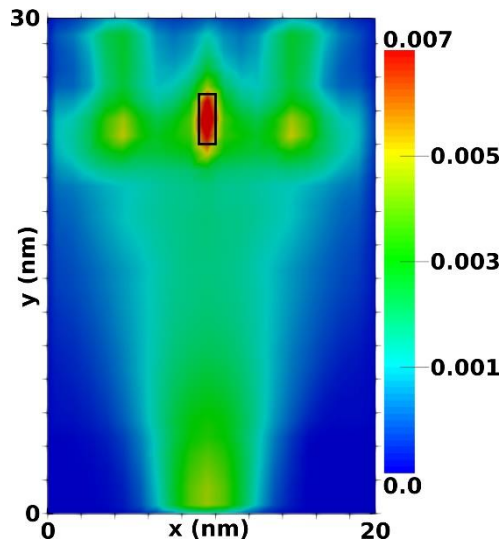


Fig. 3: Kill zone density distribution (arbitrary unit) after 200 fs . The black rectangle indicates the kill zone.

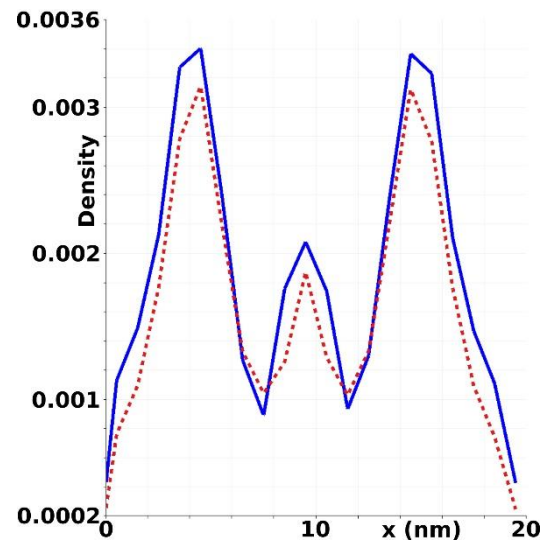


Fig. 4: Comparison of density distribution (arbitrary unit) via a screen at $y = 29 \text{ nm}$ after 200 fs .

The financial support by the Austrian Science Fund (FWF) project P29406, the EC SUPERAID7 project 688101, the Bulgarian NSF project FNI I 02/20, the Austrian Federal Ministry of Science, Research and Economy, and the National Foundation for Research, Technology and Development is gratefully acknowledged. The computational results presented have been achieved using the Vienna Scientific Cluster (VSC).