The Influence of Electrostatic Lenses on Wave Packet Dynamics

Paul Ellinghaus(✉), Mihail Nedjalkov, and Siegfried Selberherr

Institute for Microelectronics, TU Wien, Vienna, Austria
{ellinghaus,nedjalkov,selberherr}@iue.tuwien.ac.at

Abstract. The control of coherent electrons is becoming relevant in emerging devices as (semi-)ballistic transport is observed within nanometer semiconductor structures at room temperature. The evolution of a wave packet – representing an electron in a semiconductor – can be manipulated using specially shaped potential profiles with convex or concave features, similar to refractive lenses used in optics. Such electrostatic lenses offer the possibility, for instance, to concentrate a single wave packet which has been invoked by a laser pulse, or split it up into several wave packets. Moreover, the shape of the potential profile can be dynamically changed by an externally applied potential, depending on the desired behaviour. The evolution of a wave packet under the influence of a two-dimensional potential – the electrostatic lens – is investigated by computing the physical densities using the Wigner function. The latter is obtained by using the signed-particle Wigner Monte Carlo method.

1 Introduction

Analogies often serve as a source of inspiration to advance research in science and technology. An example is the electrostatic lens, inspired by concepts from geometrical optics, which can be used to steer and control coherent electrons. The term *electrostatic lens* refers to a specially shaped potential with convex/concave features, as found in optical lenses, used to steer electron waves. The concept was first demonstrated experimentally in 1990 in [1,2], in low-temperature, high-mobility semiconductors, which ensured that the coherent electrons had a sufficiently long mean free path to conduct experiments with structures made with the lithographic capabilities at the time. The astounding decrease of the feature sizes in semiconductor devices, along with novel materials like graphene, has made (semi-)ballistic electron transport applicable at room temperatures [3]. This has sparked new interest in applying concepts from optics in semiconductors: electrons can be guided in a channel using total internal reflection as in optical fibres [4] or focused towards the centre of nanowires, using electrostatic lenses, to increase their mobility by avoiding rough interfaces [5].

Scanning probe microscopy allows the flow of coherent electrons in semiconductor structures to be measured and visualized with a subnanometer resolution [6,7], however, a concurrent temporal resolution to visualize dynamics on the femtosecond time scale still remains out of reach [8]. Computer simulations

I. Lirkov et al. (Eds.): LSSC 2015, LNCS 9374, pp. 277–284, 2015.
DOI: 10.1007/978-3-319-26520-9_30

can provide insight into the temporal dynamics of wave packets, which capture the physics of single electrons in mesoscopic structures. Here, we apply the two-dimensional (2D) Wigner Monte Carlo method to demonstrate its suitability as a simulation tool to investigate wave packet dynamics in the context of electrostatic lenses (and beyond).

The Wigner formalism [9] has re-emerged in recent times as a convenient formalism to consider quantum mechanical phenomena on the mesoscopic scale, since semi-classical transport models can be augmented to the coherent quantum evolution. Multi-dimensional simulations have been made computationally feasible by the signed-particle Wigner Monte Carlo method, as described in Sect. 2. Section 3 shows examples of electrostatic lenses, and their influence on the behaviour of wave packets.

2 Wigner Monte Carlo Method

The Wigner formalism expresses quantum mechanics, normally formulated with the help of wave functions and operators, in terms of functions and variables defined in the phase-space. This reformulation in the phase-space facilitates the reuse of many classical concepts and notions.

The Wigner transform of the density matrix operator yields the Wigner function, $f_w(x,p)$, which is often called a quasi-probability function as it retains certain properties of classical statistics, but the negative values which appear demand a different interpretation than the classical probability [10]. The associated evolution equation for the Wigner function follows from the von Neumann equation for the density matrix, which for the illustrative, one-dimensional case is written as

$$\frac{\partial f_w}{\partial t} + \frac{p}{m^*}\frac{\partial f_w}{\partial x} = \int dp' V_w(x, p-p') f_w(x, p', t) \,. \tag{1}$$

If a finite coherence length is considered, the implications and interpretation of which is discussed in [11,12], the semi-discrete Wigner equation result, the momentum values are quantized by $\Delta k = \frac{\pi}{L}$, and the integral is replaced by a summation. Henceforth, the index q refers to the quantized momentum, i.e. $p = \hbar(q\Delta k)$.

Equation (1) is reformulated as an adjoint integral equation (Fredholm equation of the second kind) and is solved stochastically using the particle-sign method [13]. The latter associates a $+$ or a $-$ sign to each particle, which carries the quantum information of the particle. Furthermore, the term on the right-hand side of (2) gives rise to a particle generation term in the integral equation; the statistics governing the particle generation are given by the Wigner potential (i.e. the kernel of the Fredholm equation), which is defined here as

$$V_w(x,q) \equiv \frac{1}{i\hbar L}\int_{-\frac{L}{2}}^{\frac{L}{2}} ds\, e^{-i2q\Delta k\cdot s}\left\{V(x+s) - V(x-s)\right\}. \tag{2}$$

A generation event entails the creation of two additional particles with complementary signs and momentum offsets q' and q'', with respect to the momentum q of the generating particle. The two momentum offsets, q' and q'', are determined by sampling the probability distributions $V_w^+(x, q)$ and $V_w^-(x, q)$, dictated by the positive and negative values of the Wigner potential in (2), respectively:

$$V_w^+(x, q) \equiv \max(0, V_w); \tag{3}$$

$$V_w^-(x, q) \equiv \min(0, V_w). \tag{4}$$

The generation events occur at a rate given by

$$\gamma(x) = \sum_q V_w^+(x, q), \tag{5}$$

which typically lies in the order of $10^{15}\,\mathrm{s}^{-1}$ in numerical experiments where potential differences in the order of 100 meV are encountered. This rapid increase in the number of particles makes the associated numerical burden become computationally debilitating, even for simulation times in the order of femtoseconds.

The notion of particle annihilation is used to counteract the exponential increase in the number of particles, due to particle generation [14]. This concept entails a division of the phase space into many cells – each representing a volume $(\Delta x \Delta k)$ of the phase space – within which particles of opposite sign annihilate each other. This is justified since particles of opposite sign, within the same cell, have the same probabilistic future – their contribution to the calculation of any physical quantity would be equal in magnitude, yet opposite in sign.

3 Electrostatic Lenses

The following experiments consider a minimum-uncertainty wave packet, which captures both the particle- and wave-like physical characteristics of an electron. The associated Wigner function representing this initial condition is given by

$$f_w(\mathbf{x}, \mathbf{q}) = \mathcal{N} e^{-\frac{(\mathbf{x}-\mathbf{x_0})^2}{\sigma^2}} e^{-(\mathbf{q}\Delta k - \mathbf{k_0})^2 \sigma^2}, \tag{6}$$

where $\mathbf{x_0}$ and $\mathbf{k_0}$ are two-dimensional vector quantities representing the mean position and the mean wavevector, respectively; σ is the standard spatial deviation and $\mathcal{N}$ represents a normalization constant. The wave packet travels in a two-dimensional plane towards a potential barrier, which forms the electrostatic lens. This setup is representative of a physical system where a 2D electron gas is formed at the interface between two semiconductors, e.g. GaAs/AlGaAs; the potential barrier can be induced by an appropriately shaped gate contact at the surface of the semiconductor (parallel to the interface).

A law of refraction, equivalent to Snell's law in optics, can be derived for electrostatic lenses by considering the principle of energy conservation. A particle with a wavevector $\mathbf{k}$ has a kinetic energy

$$E_k = \frac{\hbar^2 |\mathbf{k}|^2}{2m^*}, \tag{7}$$

which is reduced as the particle transverses the potential step, while its potential energy increases. The change in kinetic energy is attributed only to a change of the momentum component normal to the interface; the momentum component parallel to the lens interface (potential step) is maintained, therefore

$$|\mathbf{k}| \sin\theta = |\mathbf{k}'| \sin\theta', \tag{8}$$

where θ (θ') is the angle of incidence (transmission) with respect to the normal (of the interface) and **k**' is the wavevector of the particle within the lens region. The law of refraction follows:

$$\frac{\sin\theta'}{\sin\theta} = \frac{|\mathbf{k}|}{|\mathbf{k}'|} = \frac{\sqrt{E_k}}{\sqrt{E_k'}}. \tag{9}$$

Therefore, the square root of the kinetic energy of a particle is analogous to the refractive index used in geometrical optics.

The interaction of a wave packet with two different electrostatic lens shapes will be investigated in the following.

3.1 Wave Packet Focusing with a Double-Concave Lens

Optical lenses typically operate in a medium (air) with a lower refractive index, where the familiar double-convex shaped lens is used to focus light. A positive potential step is used here, however, making the refractive index of the electrostatic lens lower than the surrounding regions (due to a decrease in kinetic energy). Therefore, a double-concave shaped profile is needed to form a converging lens for focusing the wave packet. The potential shape used to form the electrostatic lens is shown in Fig. 1 along with the corresponding generation rate. The free evolution of a wave package is compared to the case where it interacts with the proposed lens in Fig. 2. The electrostatic lens has a peak potential of 0.04 eV and the wave packet is initialized with a kinetic energy of

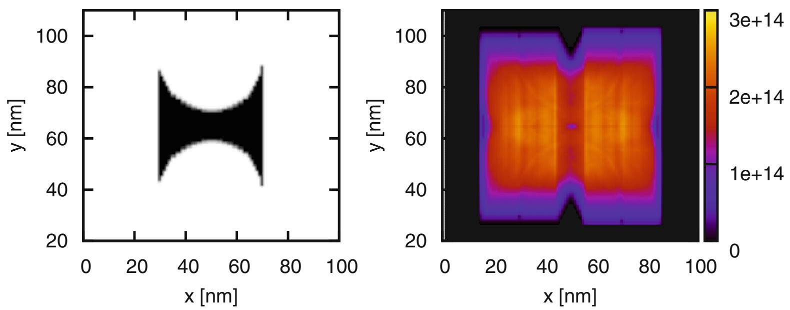
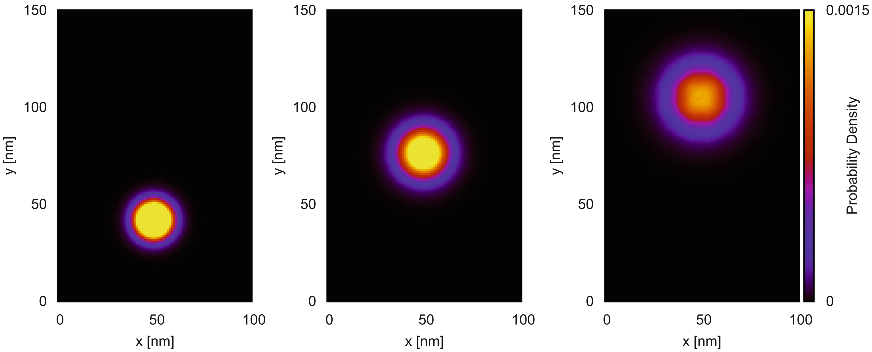
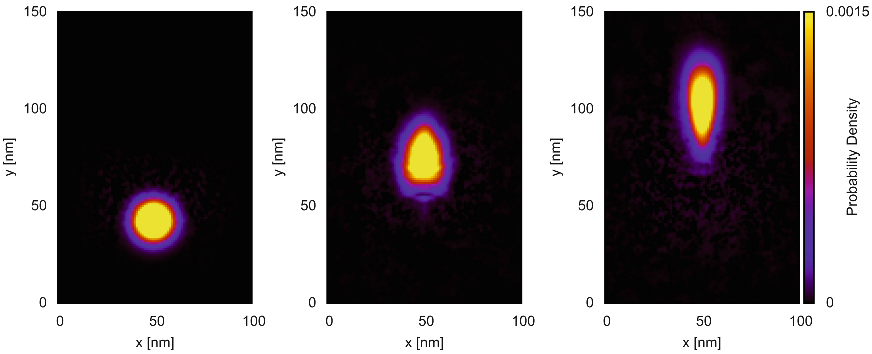


Fig. 1. Two-dimensional potential (represented in black) with a double-concave shape forming a converging electrostatic lens for electrons propagating in the y-direction. The potential value of the lens is constant; it has no three-dimensional features. The corresponding particle generation rate γ is shown on the right.



(a) 0 meV

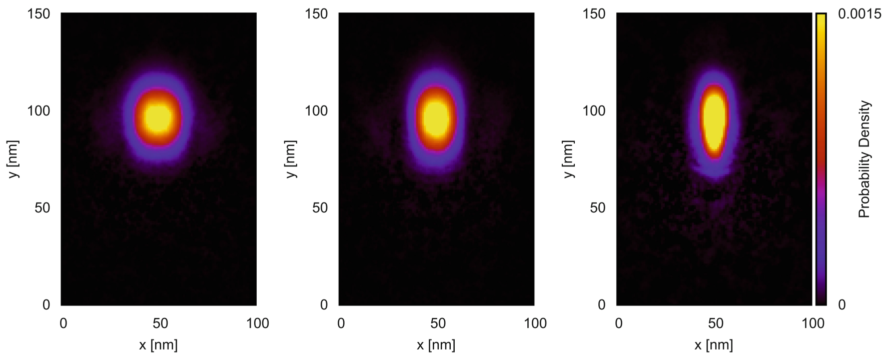


(b) 40 meV

Fig. 2. Wave packet evolving freely (top sequence) and interacting with a double concave electrostatic lens (bottom sequence); the time steps (from left to right) correspond to 40 fs, 100 fs and 150 fs.

0.18 eV, moving upwards. The electrostatic lens clearly focuses the wave packet (density) after 150 fs of evolution, compared to the case without a lens. If such a lens is added within a quantum wire (say), the focused wave packet suffers less from the surface roughness at the boundaries when compared to the spread-out wave packet in the case without a lens.

The refractive index of the lens, and thereby its focal length, can be modified by varying the magnitude of the potential with which it is formed. Figure 3 compares the effect of different potential values: It can be clearly seen that the higher potential focuses the wave packet more sharply (at the distance observed at the time instance shown). The applied potential can thereby control, when and at which distance, a wave packet is focused (on a detector, for instance).



(a) 10 meV (b) 20 meV (c) 40 meV

Fig. 3. Comparison of the density of a wave packet evolved for 135 fs in the presence of an electrostatic lens (Fig. 1) at various potential values to show different focussing.

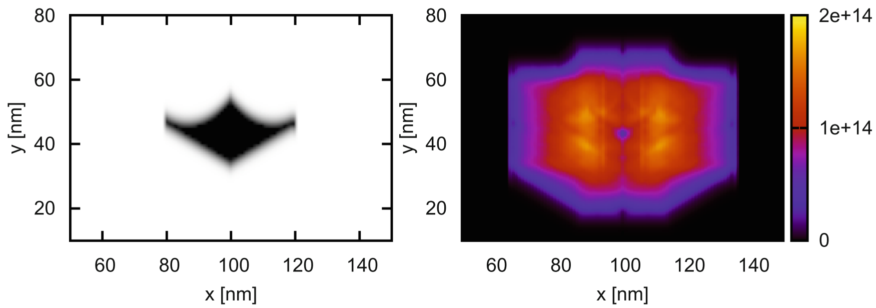
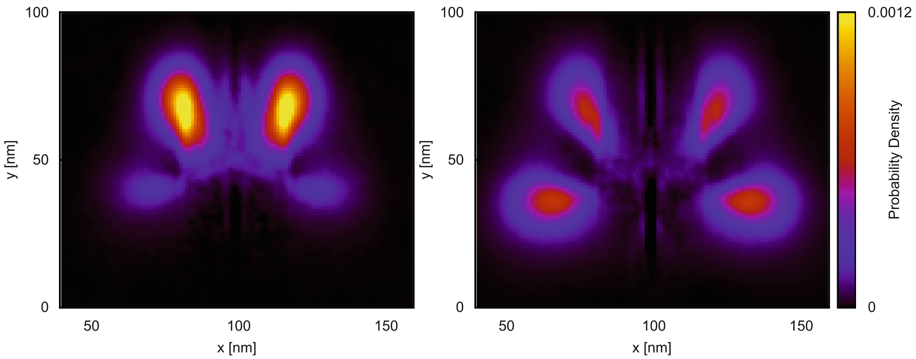


Fig. 4. Two-dimensional potential (left) with rhomboid-like shape and concave-shaped rear edges, forming an electrostatic lens to scatter an electron wave packet in various directions. The potential value of the lens is constant; it has no three-dimensional features. The corresponding particle generation rate γ is shown on the right.

3.2 Wave Packet Splitting with a Rhomboid-Like Potential

An electrostatic lens can also be used to split a wave packet into parts. Figure 4 shows a rhomboid-like potential, along with the corresponding generation rate, which forms a lens to perform such a splitting. Figure 5 illustrates the effect of the lens at different potential values. It should be noted that the electron is not split; it is a single electron in an entangled state. The density peaks indicate regions with a higher probability to find an electron. In Fig. 5a (peak potential 70 meV) the wave packet is almost fully transmitted and split into two parts. The same lens shape, but with a potential of 120 meV, splits the wave packet into four parts (Fig. 5b): The front edges splits off a portion of the wave packet by reflection, while the concave-shaped rear edges focus the transmitted parts again. In the first case, with two peaks (the most-probable components of the state), the y-component of the wavevector remains positive, whereas for the second case,



(a) 70 meV (b) 120 meV

Fig. 5. Wave packet is split either (a) into two or (b) into four parts, after 90 fs evolution, by a rhomboid-like potential profile with concave rear edges with a peak potential of 70 meV and 120 meV, respectively.

at a higher potential, the wavevector of the scattered state also has a negative y-component. This example clearly illustrates how specially shaped potentials can be used to influence the scattering pattern of an electron wave packet. By varying the potential the electron can be guided in a certain direction with a controllable probability. This can be of use in the field of quantum computing to generate a (modifiable) entangled state and direct it to other computing elements.

4 Conclusion

It has been shown that 2D Wigner Monte Carlo simulations, using the signed-particle method, can be applied to investigate the dynamics of wave packets interacting with electrostatic lenses formed in mesoscopic semiconductor structures. The concept of electrostatic lenses enables the control of coherent electrons by focusing or splitting wave packets in a controllable fashion. This ability can be utilized in emerging mesoscopic semiconductor devices, where (semi-)ballistic transport at room temperature becomes feasible.

Acknowledgement. This work was partially supported by the Bulgarian NSF under the grant DFNI 02/20.

References

1. Spector, J., Stormer, H.L., Baldwin, K.W., Pfeiffer, L.N., West, K.W.: Electron focusing in two-dimensional systems by means of an electrostatic lens. Appl. Phys. Lett. **56**(13), 1290–1292 (1990)
2. Sivan, U., Heiblum, M., Umbach, C.P., Shtrikman, H.: Electrostatic electron lens in the ballistic regime. Phys. Rev. B **41**, 7937–7940 (1990)

3. Wang, R., Liu, H., Huang, R., Zhuge, J., Zhang, L., Kim, D.W., Zhang, X., Park, D., Wang, Y.: Experimental investigations on carrier transport in Si nanowire transistors: ballistic efficiency and apparent mobility. IEEE Trans. Electron Devices **55**(11), 2960–2967 (2008)
4. Williams, J.R., Low, T., Lundstrom, M.S., Marcus, C.M.: Gate-controlled guiding of electrons in graphene. Nat. Nanotechnol. **6**(4), 222–225 (2011)
5. Muraguchi, M., Endoh, T.: Size dependence of electrostatic lens effect in vertical MOSFETs. Jpn. J. Appl. Phys. 53(4S), 04EJ09 (2014)
6. LeRoy, B.J.: Imaging coherent electron flow. J. Phys. Condens. Matter **15**(50), R1835 (2003)
7. Sellier, H., Hackens, B., Pala, M.G., Martins, F., Baltazar, S., Wallart, X., Desplanque, L., Bayot, V., Huant, S.: On the imaging of electron transport in semiconductor quantum structures by scanning-gate microscopy: successes and limitations. Semicond. Sci. Technol. **26**(6), 064008 (2011)
8. Loth, S., Burgess, J.A.J., Yan, S.: Scanning probe microscopy: close-up on spin coherence. Nat. Nanotechnol. **9**(8), 574–575 (2014)
9. Wigner, E.: On the quantum correction for thermodynamic equilibrium. Phys. Rev. **40**, 749–759 (1932)
10. Leibfried, D., Pfau, T., Monroe, C.: Shadows and mirrors: reconstructing quantum states of atom motion. Phys. Today **51**(4), 22–28 (1998). Print edition
11. Ellinghaus, P., Nedjalkov, M., Selberherr, S.: Implications of the coherence length on the discrete Wigner potential. In: 2014 International Workshop on Computational Electronics (IWCE), pp. 1–3 (2014)
12. Nedjalkov, M., Vasileska, D.: Semi-discrete 2D Wigner-particle approach. J. Comput. Electron. **7**(3), 222–225 (2008)
13. Nedjalkov, M., Schwaha, P., Selberherr, S., Sellier, J.M., Vasileska, D.: Wigner quasi-particle attributes - an asymptotic perspective. Appl. Phys. Lett. **102**(16), 163113 (2013)
14. Sellier, J.M., Nedjalkov, M., Dimov, I., Selberherr, S.: The role of annihilation in a Wigner Monte Carlo approach. In: Lirkov, I., Margenov, S., Waśniewski, J. (eds.) LSSC 2013. LNCS, vol. 8353, pp. 186–194. Springer, Heidelberg (2014)