



## Toward solotronics design in the Wigner formalism



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### HIGHLIGHTS

- We propose a honeycomb structure made of dopants only.
- We apply the Wigner Monte Carlo method based on signed particles to perform a time-dependent study of electron transport.
- We depict the conditions under which a honeycomb structure behaves as a well-transmitting ballistic channel.
- We observe the creation and destruction of symmetries in the traveling wave-packet.

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### ABSTRACT

The capability of manipulating single dopant atoms in semiconductor materials, with atomic precision, has given birth to a new branch of electronics known as solotronics (solitary dopant optoelectronics). While experiments are advancing rapidly, the theoretical comprehension of quantum phenomena occurring at that scale is relatively basic. Indeed, in this context, simulations come with incredible mathematical challenges. This eventually prevents practical design and optimization of solotronic devices. In this work, we focus our attention on a planar honeycomb structure exploiting single dopants embedded in silicon and study under which conditions it behaves as an electron ballistic channel. To this aim, we apply the time-dependent Wigner Monte Carlo formalism, based on signed particles to simulate and analyze the phenomena occurring in the proposed structure. We show that, by positioning the dopant atoms (phosphorus and boron) in particular planar patterns (honeycomb), it is possible to control the dynamics of a single electron. Finally, by introducing spatial distortions, we can show how the time-dependent electron dynamics is eventually affected. The results confirm that the Wigner Monte Carlo method is an efficient TCAD (Technology Computer Aided Design) tool which can be exploited for the time-dependent simulation of even more realistic situations necessary for the design of active solotronic devices.

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## 1. Introduction

Since the birth of semiconductor research, dopant atoms have played an important role in the comprehension and design of functioning devices. For instance, in the early days it was difficult to duplicate measurements due to the ubiquity of unintentional dopants. Several decades later, the purity of germanium is better than 1 part in  $10^{11}$ , and a similar level of purity can be obtained for silicon [1]. Thus, nowadays it is possible to have absolutely pure semiconductor materials on a nanometer scale. Even more interestingly, experimental techniques now exist which can position dopants with atomic precision and address a single atom at a time in semiconductor materials. Indeed, by using a scanning tunneling microscope (STM) in

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ultrahigh vacuum environment, it is possible to select one atom of silicon and substitute it with an atom of dopant [2–7], i.e. a complete fabrication process is available for the creation of robust devices at the nano and atomic scale. This offers new degrees of freedom to experimentalists and engineers, opening the way to solitary dopant optoelectronics, or in other words, solotronics. Therefore it is not surprising that, recently, the International Technology Roadmap for Semiconductors (ITRS) has underlined the importance of developing a three-dimensional electronic transport simulator able to include, in a reliable fashion, the effects of single dopant atoms [8].

This represents a profound departure from the CMOS (complementary metal–oxide–semiconductor) technology but it also is an opportunity for the development of drastically different device architectures. In particular, among the many possible solotronic instances, a new class of Silicon based devices exploiting single dopant atoms have been proposed [9]. The experiments are advancing quite quickly [10,11], but the theoretical comprehension still remains elementary due to the incredible mathematical challenges posed by the simulation requirements. As a matter of fact, a meaningful study of solotronic design requires a time-dependent, full quantum, and multi-dimensional model, even in the relatively simpler case of ballistic regime. Eventually, the lack of such TCAD (Technology Computer Aided Design) tools prevents practical design and optimization of realistic solotronic devices.

From this perspective, the Wigner equation [12] appears to be very promising. It is indeed a time-dependent, full quantum and multi-dimensional model which is intuitive (it is based on the concept of a quasi-distribution function defined in the phase-space) and totally equivalent to the Schrödinger model (through the invertible Wigner–Weyl transform). Despite the numerical difficulties imposed by such a partial integro-differential equation, a Monte Carlo (MC) technique exists enabling practical simulations of the Wigner equation based on (virtual) signed particles [13]. This method relies on the Iterative MC technique [14,15], a time-dependent approach for partial differential equations which can deal with general initial and boundary conditions. It has already been applied successfully to the study of arrays of dopants, a problem close to solotronics [16].

In this work, we propose several different arrangements of phosphorus and boron atoms forming planar honeycomb structures embedded in silicon. Our aim is to study the conditions for controlled propagation of electronic wave-packets from one point to another of the spatial domain (ballistic channels). To this scope, we introduce some degree of distortion in the structures and show how the electron dynamics varies. By applying the signed particle Wigner MC method we are able to study the time-dependent evolution of an electron wave-packet inside these structures. In particular when no distortion is introduced, we show that a planar honeycomb structure, involving phosphorus dopants only, acts as a perfectly transmitting channel (it indeed transports an electron along an assigned path) while the other structures, involving phosphorus and boron dopants (scattering centers), destroys the transmission. In other words, as soon as some level of distortion is introduced, the dynamics of electrons is profoundly affected making the transmission more difficult to happen.

This work is twofold. On one side, we propose four different solotronic arrangements of dopants and show under which conditions honeycomb structures embedded in very thin silicon films can be used as ballistic channels to propagate one or more electrons between two points of a semiconductor substrate in a controlled manner. On the other side, we show how the Wigner MC method can be applied to practical technology relevant cases giving a time-dependent perspective on the occurring quantum phenomena. Indeed, the same simulation technique could eventually be utilized to investigate more complex patterns of dopant atoms to design active solotronic devices such as single electron transistors.

## 2. The Wigner Monte Carlo technique

In this section, we briefly outline the essential concepts involved in the Wigner MC method. More details can be found in Refs. [13–15] where a complete description of the technique and its implementation is given.

In a two-dimensional (2D) space, corresponding to a four-dimensional (4D) continuous phase-space, the Wigner model is a partial integro-differential equation which reads

$$\frac{\partial f_W}{\partial t} + \frac{p_x}{m} \frac{\partial f_W}{\partial x} + \frac{p_y}{m} \frac{\partial f_W}{\partial y} = Q_W[f_W], \quad (1)$$

where  $f_W = f_W(x, y, p_x, p_y, t)$  is the unknown quasi-distribution function defined over the phase-space  $(x, y, p_x, p_y)$ ,  $m$  is the mass of an electron, and  $Q_W$  is the functional defined over the space of quasi-distributions

$$Q_W[f_W](x, y, p_x, p_y, t) = \int dp'_x dp'_y V_W(x, y, p_x - p'_x, p_y - p'_y, t) f_W(x, y, p'_x, p'_y, t).$$

Finally, the function  $V_W = V_W(x, y, p_x, p_y, t)$  known as the Wigner kernel (or, sometimes, Wigner potential) is defined as

$$V_W(x, y, p_x, p_y, t) = \frac{1}{i \hbar^2 2\pi} \int dx' dy' e^{-i \frac{p_x x' + p_y y'}{\hbar}} \left[ V \left( x + \frac{x'}{2}, y + \frac{y'}{2}, t \right) - V \left( x - \frac{x'}{2}, y - \frac{y'}{2}, t \right) \right]. \quad (2)$$

By discretizing the space of momenta  $\Delta p_{x/y} = \frac{\hbar\pi}{L_c^{x/y}}$  (where  $L_c^{x/y}$  is a free parameter defining the momentum step), one can rewrite accordingly the Wigner equation in a semi-discrete fashion [13]. The space of momenta being now expressed in terms of multiples of the quantity  $\Delta p$ , a momentum can be denoted as a couple of integers  $(M, N)$  with  $p_x = M \Delta p_x$  and

$p_y = N \Delta p_y$ . Thus, the Wigner equation now reads

$$\begin{aligned} & \frac{\partial f_W}{\partial t}(x, y, M, N) + \frac{M \Delta p_x}{m} \frac{\partial f_W}{\partial x}(x, y, M, N) + \frac{N \Delta p_y}{m} \frac{\partial f_W}{\partial y}(x, y, M, N) \\ & = \sum_{M'=-\infty}^{+\infty} \sum_{N'=-\infty}^{+\infty} V_W(x, y, M - M', N - N') f_W(x, y, M', N'), \end{aligned} \quad (3)$$

where the semi-discrete Wigner kernel becomes

$$V_W(x, y, M, N, t) = \frac{1}{i \hbar^2 L_C^x L_C^y} \int_{-L_C^x/2}^{L_C^x/2} dx' \int_{-L_C^y/2}^{L_C^y/2} dy' e^{\left(-i \frac{M \Delta p_x x' + N \Delta p_y y'}{\hbar}\right)} [V(x + x', y + y', t) - V(x - x', y - y', t)].$$

We can, thus, apply the Iterative MC method [14,15] to the semi-discrete Wigner equation (3) and achieve reliable time-dependent simulations of the system [13]. By introducing the quantity  $\gamma = \gamma(x, y)$  (obtained from the Wigner kernel, see Ref. [13]), it is possible to define a particle generation process, where all particles carry a sign (positive or negative). During its field-less flight, a signed parent particle creates a pair of new particles, one positive and the other negative, ending up with three particles. In particular, if the parent particle started with a sign  $s$ , position  $(x, y)$  and momenta  $(M, N)$ , it generates a pair of new particles with signs  $s, -s$  and momenta  $(M + M', N + N'), (M - M', N - N')$  respectively, in the same position of the parent particle, with a change in momenta provided by the Wigner kernel [13]. Then, the parent particle continues its flight until a given time  $T$  and the new pair of particles is evolved in turn. All signed particles contribute to the values of the physical averages only by their sign. In particular, the negative signed particles contribute to the negative part of the Wigner quasi-distribution function, a clear signature of the presence of quantum effects.

This method has been validated against multi-dimensional benchmark tests and technologically relevant situations [13,16,17].

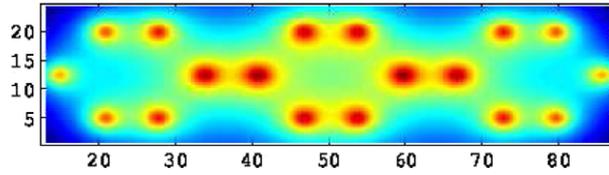
### 3. Numerical experiments

In this section, we propose four different arrangements of dopant atoms behaving as channels for electrons at the nanometer scale, where in the last two patterns some degree of controlled distortion is introduced in the structure. This is twofold. First, we present possible solotronics channels made only by arranging dopant atoms on a plane buried in a silicon substrate, and which may be used for moving electrons from one point to another of the substrate. Indeed, we show that, by exploiting a honeycomb arrangement, these structures can reproduce, under certain conditions, the electric features of well-tempered ballistic channels which essentially transport one electron from one point to another of a given spatial domain. Second, this clearly demonstrates that the Wigner MC method can be utilized concretely for solotronic engineering design. As a matter of fact, all simulations performed are time-dependent which enables a realistic visualization of the phenomena happening in nanometric structures and, thus, a higher level of details. This is a result hardly achievable with other formalisms such as the Keldysh one, where the Kadanoff–Baym equation still remains a daunting task for the actual computational resources [18,19]. Obviously, one should note that the method introduced in this section represents the first approach to the problem of simulating more complex situations involving active devices. Indeed, in this case, a more realistic technique should involve the use of the Poisson equation coupled to the Wigner equation in a self-consistent way. From these experiments, anyway, it becomes clear how one could eventually use the Wigner MC approach to design more sophisticated (active) devices such as single electron transistors.

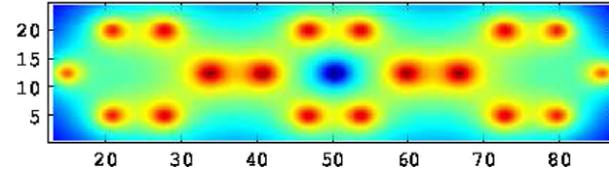
#### 3.1. Structures and model

The four numerical experiments performed in this section consist of planar dopant honeycomb structures (Figs. 1 and 2) and their distorted counterparts (Figs. 3 and 4) embedded in a 2D Silicon box with dimensions  $L_x = 100 \text{ nm} \times L_y = 25 \text{ nm}$ . We explored several types of dopant arrangements until we realized, by means of Wigner simulations, that the honeycomb structure seems to be the most convenient for our purpose. We also have noticed how distortions can play an important role in the dynamics of an electron moving through the structure. In particular, Fig. 1 shows a structure made of phosphorus dopants only (positive charges). Fig. 2 shows, instead, a structure made of phosphorus atoms but one boron atom (repulsive charge) is positioned in the middle of the domain (negative Coulombic potential). Finally, Fig. 3 shows a distorted version of the structure reported in Fig. 1, and Fig. 4 shows a structure similar to the one reported in 2 where the boron atom is now off-centered.

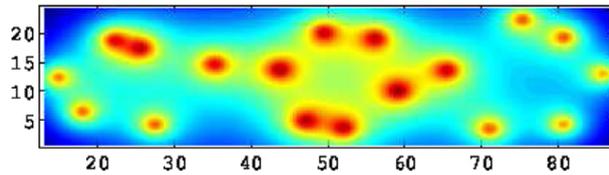
For all experiments, the left-hand side and right-hand side boundaries are absorbing, while the top and bottom are reflective walls (these conditions are in agreement with Ref. [20] which requires time-irreversibility at the contacts). A initial Gaussian wave packet (Fig. 5), with a purely longitudinal momentum (directed from left to right), is evolved in time till a final time equal to 250 fs is reached. The imposed initial conditions do not represent a restriction for the method and more sophisticated (realistic) conditions could be used, as suggested in Refs. [21,22] where the use of planar waves injected by the contacts is discussed.



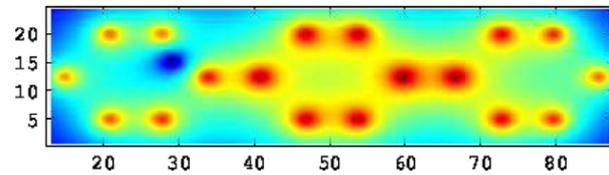
**Fig. 1.** Electrostatic potential generated by a honeycomb structure made of phosphorus atoms only. This structure behaves as a ballistic channel. Coordinate dimensions are in nanometer.



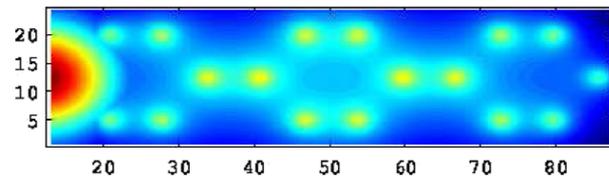
**Fig. 2.** Electrostatic potential generated by a phosphorus (positive charges) honeycomb structure with a boron atom (negative charge) in the center of the domain. Coordinate dimensions are in nanometer.



**Fig. 3.** Electrostatic potential generated by a distorted phosphorus honeycomb structure. Coordinate dimensions are in nanometer.



**Fig. 4.** Electrostatic potential generated by a phosphorus (positive charges) honeycomb structure with a off-centered boron atom (negative charge). Coordinate dimensions are in nanometer.



**Fig. 5.** Initial conditions for a Gaussian wave packet in a wire made of phosphorus dopants in the honeycomb structure.

The Coulombic potential, representing the  $i$ th dopant atom, is mathematically expressed as

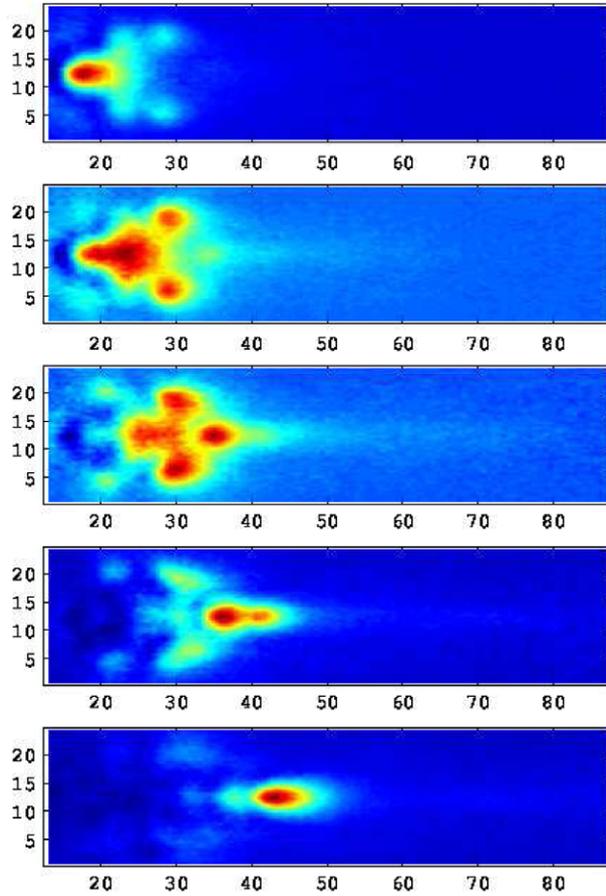
$$V_i(x, y) = \frac{q}{4\pi\epsilon_0\epsilon_r \left( (x - x_i)^2 + (y - y_i)^2 + \frac{1}{2}a_0^2 \right)^{\frac{1}{2}}}, \quad (4)$$

where  $a_0$  is the Bohr radius in silicon  $a_0 = \frac{4\pi\epsilon_0\epsilon_r\hbar^2}{m^*e^2}$  [23] and  $(x_i, y_i)$  is the position of the center of the  $i$ th dopant. This model has been extensively validated [23] and has been extended to the Wigner MC method in Ref. [16]. Clearly, the choice of this truncated Coulombic potential is not a restriction and any other potential can be used.

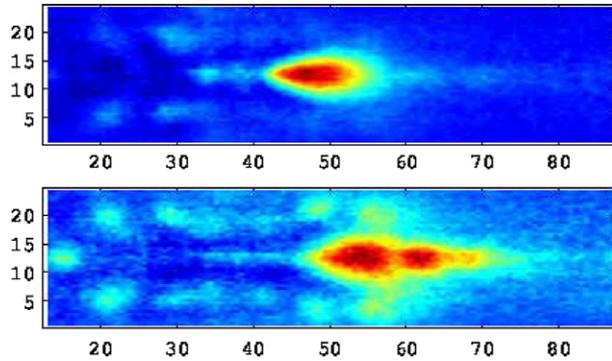
Finally, we extend the Ramo–Shockley theorem to the case of signed particles in the context of the Wigner MC method. Now, the current  $I$  measured through a contact is equal to:

$$I = -\frac{q}{L} \sum_i s_i v_i, \quad (5)$$

where  $q$  is the elementary charge,  $L$  is the dimension of the contact, and  $s_i$  and  $v_i$  are the sign and the transversal (with respect to the contact) component of the velocity of the  $i$ th virtual particle respectively. In a broad sense, this generalization



**Fig. 6.** Evolution in time of a wave packet in a phosphorus only honeycomb structure. The packet moves from one lead (left-hand side) to the other (right-hand side). The plots correspond to times equal to 50 fs, 70 fs, 90 fs, 110 fs and 140 fs respectively.

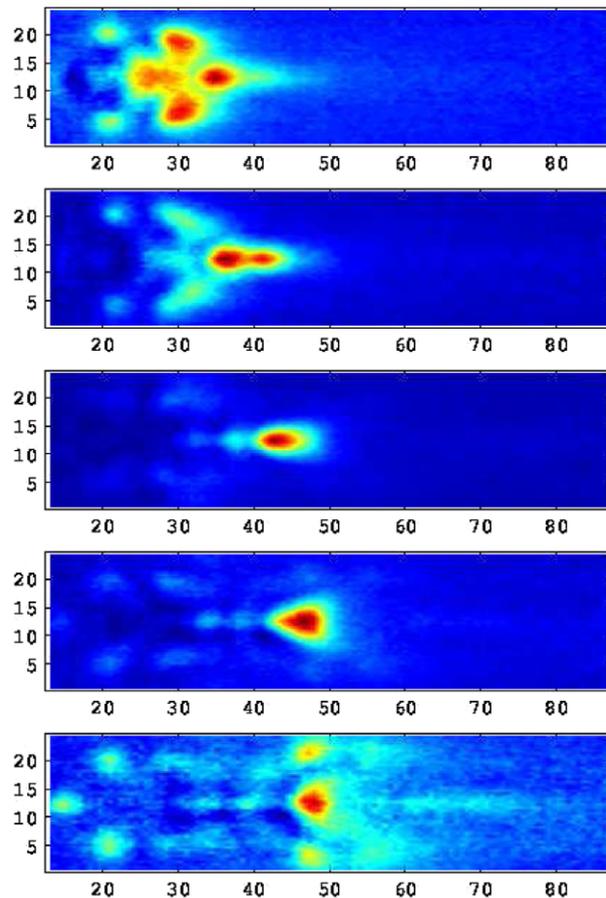


**Fig. 7.** Evolution in time of a wave packet in a phosphorus only honeycomb structure. The packet moves from one lead (left-hand side) to the other (right-hand side). The plots correspond to times equal to 170 fs and 200 fs respectively.

is similar to the one for the Wigner MC method based on the concept of quantum affinity [24]. We will make use of this formula to create a connection between the results of our simulations and the possible outcomes of physical experiments.

### 3.2. Phosphorus honeycomb channel

The simulation results concerning a phosphorus arrangement (see Fig. 1) behaving as a perfectly transmitting ballistic channel are reported in Figs. 6 and 7. The plots of Fig. 6 (from top to bottom) show the time-dependent evolution of an electron wave-packet at time 50 fs, 70 fs, 90 fs, 110 fs and 140 fs respectively while Fig. 7 shows the evolution at times 170 fs and 200 fs respectively. Initially the wave-packet collapses into the first encountered phosphorus dopant (at about



**Fig. 8.** Evolution in time of a wave packet in a dopant honeycomb structure with a scattering center in the middle of the domain. The packet moves from one lead (left-hand side) to the other (right-hand side) until it starts to feel the effects of the boron atom. The plots correspond to times equal to 90 fs, 110 fs, 140 fs, 170 fs and 200 fs respectively.

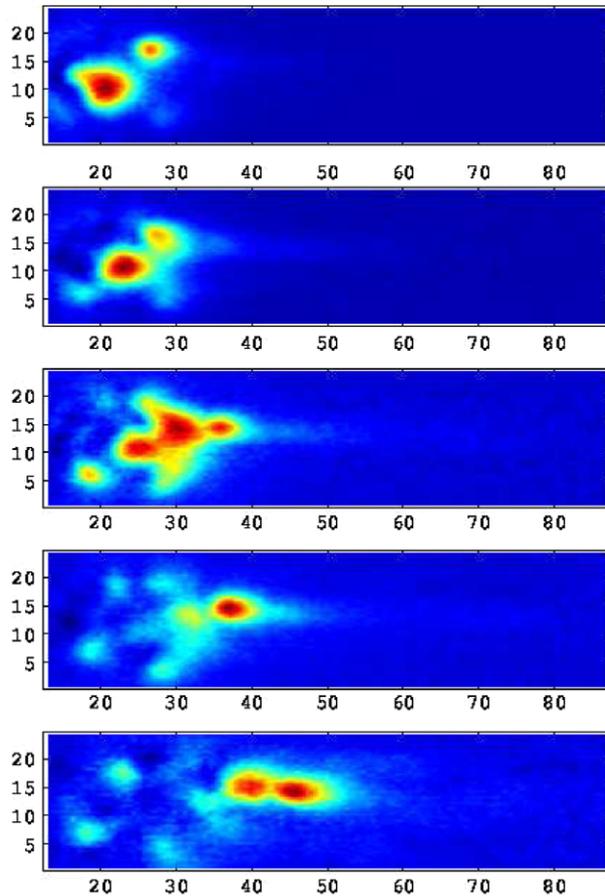
50 fs). Being the electron energetic enough, it proceeds in its initial direction toward the other dopants splitting into three main pieces (at about 70 fs). The evolution proceeds in several pieces (90 fs) until a phosphorus dopant is encountered in the middle of the domain (110 fs). At that point, the three pieces recombine into one wave-packet and the evolution proceeds in a way similar to the one happening at 50 fs. It is clear from this experiment how a phosphorus planar honeycomb structure could be exploited to transfer an electron from one point of the domain to another (and one may even imagine to gradually bend this structure to transfer an electron in diagonal directions).

By using the Ramo–Shockley formula (5) and the simulation results concerning a phosphorus planar honeycomb pattern, it is possible to see that the current measured through the right-hand side contact is maximal if compared to the situations described below. As a matter of fact, when no scattering center is present and the honeycomb structure is not distorted, the wave packet velocity proceeds longitudinally keeping its transversal component practically equal to zero. This, in other words, means that the current is at its peak. In the next experiments, we will show that not only a scattering center can drastically affect the performances of such proposed channel, but also distortions can play a very important role.

### 3.3. Addition of a boron atom

We now add a boron atom (negative charge) at the exact center of the domain (Fig. 2). The dopant arrangement remains the same as the previous one with the only exception of the boron atom which essentially acts as a scattering center. The aim of this numerical experiment is to show that some dispersion of the wave-packet is observed and, in a broad sense, a non-linear resistor is obtained (one may also consider this fact as a further proof of the validity of the Wigner MC approach). Thus, this section shows that in order to achieve a perfect transmission through the honeycomb structure no scattering center has to be present.

The simulation results concerning this new structure are reported in Fig. 8. In particular, Fig. 8 shows the time-dependent evolution of an electronic wave-packet at 90 fs, 110 fs, 140 fs, 170 fs and 200 fs respectively. One clearly sees how the dynamics of the wave-packet is dominated by the arrangement of phosphorus dopants until time equal to 140 fs (compare



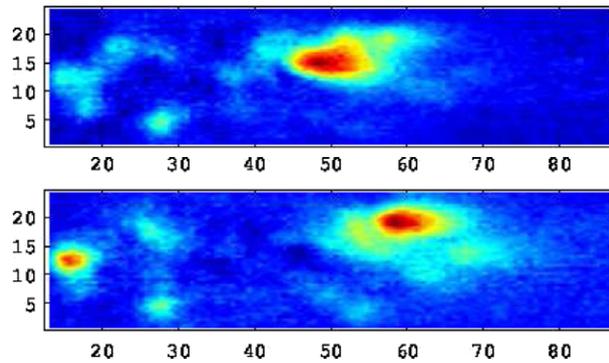
**Fig. 9.** Evolution in time of a wave packet in a distorted phosphorus honeycomb structure. The plots correspond to times equal to 50 fs, 70 fs, 90 fs, 110 fs and 140 fs respectively.

with Fig. 6). Indeed, no noticeable difference can be observed between the structure of the previous section and the one considered in this experiment in that initial period of time. Only when the wave-packet eventually starts to feel the boron atom (at about 170 fs) the dynamics changes drastically (compare with Fig. 7). As a matter of fact, one clearly notices how the wave-packet partly scatters back and partly tunnels through the Coulombic potential due to the boron atom. This time the three main contributions visible at time 90 fs do not recombine in a single wave-packet as it used to happen in the previous structure (ballistic channel). Experimentally speaking, this is equivalent to observe a decrease in electronic current at the right-hand side contact. Indeed, now the wave-packet has a strong transversal component which reduces the current calculated by means of formula (5).

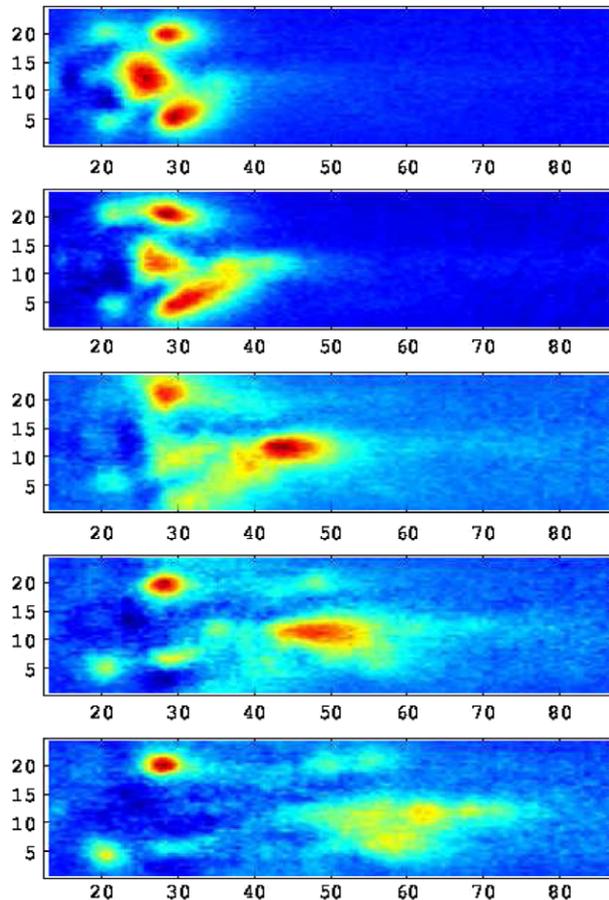
### 3.4. Distorted honeycomb structures

In this experiment, we start from the structure depicted in Fig. 1. We perturb, in a controlled manner, the position of the phosphorus dopants by adding noise in the spatial coordinates of the dopants. The final structure obtained is shown in Fig. 3. This experiment shows that a distorted honeycomb structure does not perform as well as an undistorted one.

The simulation results concerning the distorted channel are shown in Figs. 9 and 10. In particular, the plots of Fig. 6 (from top to bottom) show the time-dependent evolution of an electron wave-packet at time 50 fs, 70 fs, 90 fs, 110 fs and 140 fs respectively while Fig. 7 shows the evolution at times 170 fs and 200 fs respectively. While, it is possible to show that for small distortions the electron dynamics is essentially the same, in the case of strongly distorted honeycomb structures the evolution in time is profoundly different. Indeed, first of all we note that, if compared to Figs. 6 and 7, the wave-packet has now a transversal velocity component and it goes first upward and then downward according to the dominant spatial arrangement of the dopants. In terms of formula (5), this means a lower current measured at the right-hand side contact. Furthermore, at time 200 fs (Fig. 10) one clearly see how the probability of finding the electron is prominent in two localized areas, one of which is close to the initial position of the wave-packet (left-hand side contact). This phenomenon is not observable when the honeycomb structure is undistorted (Fig. 7). Thus, a relatively high degree of accuracy is needed when building a solotronic ballistic channel if good transmission (or equivalently high current) is the main goal.



**Fig. 10.** Evolution in time of a wave packet in a distorted phosphorus honeycomb structure. The plots correspond to times equal to 170 fs and 200 fs respectively.



**Fig. 11.** Evolution in time of a wave packet in a dopant honeycomb structure with a off-centered scattering center. The plots correspond to times equal to 90 fs, 110 fs, 140 fs, 170 fs and 200 fs respectively.

### 3.5. Off-centered boron atom

Finally, we perform a study of the time-dependent evolution of an electron wave-packet in the presence of a phosphorus honeycomb structure and a boron atom which is off-centered (Fig. 4).

The simulation results are shown in Fig. 11 for times equal to 90 fs, 110 fs, 140 fs, 170 fs and 200 fs respectively. It is now clear to see how an off-centered boron atom strongly affects the evolution of an electron wave-packet. Indeed, the packet is almost instantly destroyed by the presence of the scattering center and the probability of finding an electron remains much higher close to the initial (left-hand side) contact. In other words, not only the boron atom destroys the symmetry of the

traveling wave-packets, it also drastically reduces the current measured at the right-hand side contact. Thus, at this scale, it is important that any random scattering center is removed from the structure.

### 3.6. Software and hardware

The results presented in this section have been obtained using the HPC cluster installed at the Institute of Information and Communication Technologies (IICT) of the Bulgarian Academy of Sciences. This cluster consists of two racks which contain HP Cluster Platform Express 7000 enclosures with 36 blades BL 280c with dual Intel Xeon X5560 @ 2.8 GHz (total 576 cores), 24 GB RAM per blade. There are 8 storage and management controlling nodes 8 HP DL 380 G6 with dual Intel X5560 @ 2.8 GHz and 32 GB RAM. All these servers are interconnected via non-blocking DDR Infiniband interconnect at 20 Gbps line speed. The theoretical peak performance is 3.23 Tflops.

The simulator (nano-archimedes) used in this work is a modified version of Archimedes, the GNU package for the simulation of carrier transport in semiconductor devices [25] released for the first time in 2005 under the GNU Public License (GPL). In particular, the purpose of nano-archimedes is the simulation of quantum dynamics for one or more electrons. The code is entirely developed in C and optimized to get the best performance from the hardware. The results of the new version are posted on the nano-archimedes website [26].

## 4. Conclusions

In this paper, we have applied the Wigner Monte Carlo method, based on virtual signed particles, to the simulation of four proposed planar dopant honeycomb structures. This is twofold. First of all, we have shown how, under certain particular conditions (no distortion and no scattering center), a honeycomb structure can be used to replicate the characteristics of a well-tempered ballistic channel at the nanometer scale. One may, indeed, imagine (and design) even bended honeycomb structures creating a path for electrons between two points of a silicon substrate. Second, we have shown how the Wigner formalism can be utilized for practical design of solotronics structures. As a matter of fact, it allows full quantum, multi-dimensional and time-dependent simulations, a result hardly achievable with other formalisms which are still too demanding in terms of computational resources. In particular, in Figs. 6, 7, 8, 9, 10, and 11 we have shown the time-dependent evolution of an initially Gaussian wave packet moving in four different structures shown in Figs. 1–4, for a phosphorus honeycomb structure, a centered boron atom, a distorted honeycomb structure and an off-centered boron atom respectively. From these results, it is possible to see that planar honeycomb structures made of dopants, such as phosphorus and boron atoms, could be used to achieve practical solotronic devices under certain conditions. This demonstrates that the Wigner formalism could be utilized for more sophisticated simulations opening the way toward solotronic TCAD tools for the design of active devices exploiting single dopant atoms.

Finally, one should note that all simulations presented in this work are performed in the ballistic regime, in a non self-consistent fashion and for Gaussian wave-packets. It would be interesting to study the same structures in the presence of phonon scattering, with contacts injecting planar wave-packets, along with a self-consistent coupling to the Poisson equation. As a matter of fact, our future plan is to apply the method depicted in Ref. [27] to this novel context in order to simulate, in a realistic and reliable way, active solotronic devices such as single electron transistors.

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