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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.

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 scoper, 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

$$\frac{\partial f_W}{\partial t} + \frac{p_x}{m}\frac{\partial f_W}{\partial x} + \frac{p_y}{m}\frac{\partial f_W}{\partial y} = Q_W\left[f_W\right], \tag{1}$$

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

$$Q_W\left[f_W\right](x, y, p_x, p_y, t) = \int \mathrm{d}p'_x \mathrm{d}p'_y V_W(x, y, p_x - p'_x, p_y - p'_y, t) f_W(x, y, p'_x, p'_y, t).$$

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

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

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 Δp, a momentum can be denoted as a couple of integers (M, N) with $p_x = M\Delta p_x$ and