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Electrostatic and substrate-based monolayer graphene superlattices: Energy minibands and its relation with the characteristics of the conductance curves

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We study the transmission, transport and electronic structure properties of monolayer Graphene Superlattices (GSLs). The transfer matrix method has been implemented to obtain the transmittance, linear-regime conductance and electronic structure. In particular, we have studied two types of GSLs: (1) Electrostatic GSLs (EGSLs), structures formed with electrostatic potentials and (2) Substrate GSLs (SGSLs), obtained by alternating substrates that can open and non-open, such as SiC and SiO_2, an energy bandgap on graphene. We have found that the transmission properties can be modulated readily by changing the main parameters of the systems: well and barrier widths, energy and angle of the incident electrons and the number of periods of GSLs. In the case of the linear-regime conductance turns out that it diminishes by increasing the barrier width as well as the number of periods for SGSLs. On the contrary, Klein tunneling sustains the conductance in EGSLs. Calculating the electronic structure or miniband-structure formation we establish a direct connection between the conductance peaks and the start–end and degeneration (narrowing) of the energy minibands for EGSLs, and start–end, degeneration (narrowing) and closure in the case of SGSLs.

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1. Introduction

It is well known that periodic order appears in multiple aspects of nature as well as it can be exploited technologically [1]. For instance, periodic modulation was the instrument to unveil quantum effects in semiconductor artificial structures [2,3], giving rise to what later on was known as semiconductor superlattice. Among the most important properties of semiconductor superlattices we can find excitonic effects, miniband transport, Wannier–Stark localization, Bloch oscillations, resonant tunneling and electric field domains [1]. Most of these properties rely on the miniband structure or miniband dispersion presented in semiconductor superlattices [1–3]. So, by considering the importance of the periodic modulation, from both the fundamental and technological standpoints, it seems natural that it would be an extension for any novel material.

To this respect graphene [4–6] is not the exception, and shortly after its discovery it was subjected to an intense research, especially with regard to how its fundamental properties are modified under the influence of a periodic modulation [7–54]. There are different mechanisms or effects proposed to modulate graphene in periodical fashion, among them we can mention electric and magnetic fields [7–37], breaking-symmetry substrates [38–41], strain [42–46], hydrogenation [47–51] and disorder [52–54]. Graphene superlattice (GSL) is the term used to refer to graphene under periodic modulation, irrespective of the mechanism used to generate the periodic pattern. The effects produced by a periodic modulation in graphene are remarkably different to what we are used to see in traditional semiconductors. Firstly, the periodic pattern creates additional Dirac cones in the energy dispersion of graphene. Secondly, the propagation of charge carriers through GSL is highly anisotropic, and in some cases results in carrier velocities that are diminished to zero in one direction and are unchanged in another. The density and type of carrier species is also pretty sensitive to the periodic pattern considered. Thirdly, by changing the structure parameters of GSL (potential of barriers and wells, period of the potential and transverse wave number) the angular-averaged conductivity can be controlled readily. See for instance [7–9]. As we can corroborate above, periodic patterns in graphene have been subjected to an intense research, however there are some issues that as far as we can see are not explain at all. Specifically, we have not found a clear and concise explanation about how periodic modulation in graphene affect the oscillatory nature of the linear-regime conductance, which is, by the way, a characteristic that is mentioned in practically all works reported so far.

Within this context, the aim of the present work is to address the main characteristics of periodic systems in graphene. Specifically, we compare the transmission, transport and electronic structure properties of the mentioned systems when the barriers that constitute them are of electrostatic and breaking-symmetry-substrate character. We consider this kind of barriers because they are opposite, one (electrostatic case) in which Klein tunneling [55,56] is presented and the other (substrate case) in which it is ruled out. Following the lines of our previous work [57], the main concern of this study is to find out how periodic modulation affects the intrinsic oscillatory nature of the linear-regime conductance in graphene as well as how these oscillations are correlated with the energy level structure.

2. Methodology

As we are interested in two antagonistic multi-barrier systems like those based in electrostatic and substrate effects, we firstly show the basics of these effects on the fundamental properties of the graphene sheet. And then we will proceed with the details of the transfer matrix approach and the Landauer–Büttiker formalism.

2.1. Electrostatic field effect in graphene

In semiconductor-based devices is well known that the electric field effect plays a fundamental role due to its ability to modulate, in a very simple way, the optoelectronic and transport properties. This is possible due to the advance and sophistication of the growth and deposition techniques, specifically thanks to the deposition of metallic contacts on semiconductor structures. Graphene is not the