Numerical study of the lattice vacancy effects on the quantum transport of four-terminal graphene nanodevice

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The electronic transport properties of four-terminal graphene nanodevice have been investigated by means of the Landauer approach using tight-binding model. The effects of single vacancy and divacancy on transport properties of the electron injected into the system have been studied. The existence of single vacancy along with the magnetic field creates additional band between Landau levels, this effect is appeared by enhancing the transmission. It is also found that in the presence of divacancy with small distance, the coupling between two vacancies due “vacancy molecules”, that the bonding between these vacancies can be tuned by the magnetic field. The effect of vacancies decreases when the size of conductor region increases. The theoretical results obtained, can be a base for development in designing graphene nanodevice.

Keywords: Four-terminal graphene nanodevice, Transport properties, Vacancy, Divacancy

1 Introduction

Recently, graphene sheets were successfully isolated and demonstrated to be stable under ambient conditions. The E-k relation is linear (E=±±±±±hl vs l) for low energies near the six corners of two-dimensional hexagonal Brillouin zone, leading to zero effective mass for electrons and holes. Graphene has the ideal properties to be an excellent component of integrated circuits. It has a high carrier mobility, as well as low noise, allowing it to be used as the channel in a field-effect transistor (FET). It may be a suitable material for the construction of quantum computers using electronic circuits. The unusual transport properties of graphene arise from its linear E-K relation from low energies near the six corners of two-dimensional hexagonal Brillouin zone. Beside the high mobility and minimum conductivity, graphene displays anomalous quantum Hall effect (QHE) different from ordinary 2D conductors, with the sequence shifted by 1/2 with respect to the standard sequence. Similar to the 2D Schrödinger electrons, 2D Dirac electron states in a perpendicular uniform magnetic field B also form highly degenerated discrete Landau levels (LLs). When the magnetic flux is getting larger, these levels form the Landau sub-bands because of the Harper broadening. Most of the experimental and theoretical studies of graphene have focused on the effect of the relativistic electronic dispersion on different phenomena such as Landau level structure or quantum Hall ferromagnetism.

One of the most striking features of graphene is its very large electron mean-free path, which makes graphene an enticing material for novel electronics applications. Ballistic transport requires the sample length to be shorter than the mean free path. The mean free path in graphene is almost independent of temperature.

Experimental observed graphene has a lot of defects due to imperfect cutting. It is well-known that defect is ubiquitous in graphene and its effect on the electronic structure has been studied extensively. One of the simplest defects is “vacancy” caused by the loss of one or several nearest atoms. Vacancies are natural defects in graphene lattice and can also be externally induced by ion beam irradiation with high energy. To recognize the vacancy defects using X-ray emission spectra, the total density of states for various sizes of vacancy defects have been obtained. In addition, the vacancy formation energy using a tight-binding (TB) method and ab initio DFT-based method has been studied recently. Theoretical works have shown that vacancies induce the formation of localized states and when particle-hole symmetry is broken, localized states become resonances close to the Fermi level.

In the following, the effects of two kinds of vacancies have been analyzed, single vacancy and divacancy, in four-terminal graphene nanodevice when a perpendicular magnetic field is applied. Based on the critical role that two-dimensional four-terminal
devices have played in semiconductor nanotechnology, four-terminal graphene nanodevices should also play an important role in any graphene based electronic circuits. Due to its high electronic quality, a four-terminal graphene nanodevice has also attracted the interest of technologists who see it as a way of constructing ballistic transistors. In addition to the practical importance of these four-terminal graphene devices, these systems make a useful framework to study the effects of lattice defects on the electron transport in the device.

Our results suggests that single vacancy introduce bounding and anti-bounding state, and two close vacancies may couple to each other forming a "vacancy molecule" tanned by the magnetic field. Furthermore, when a perpendicular magnetic field is applied to the four-terminal graphene, we found the vacancy state between Landau levels. According to our results, current in the existence of vacancy in comparison with the pure case, reduces, since the vacancy state created by defect, produces additional band.

2 Theoretical Model
The system is considered as a central conductor region (C), connected to four leads L, R, B, T (see Fig. 1). The leads are formed by semi-infinite perfect ribbons, simulating four ideal leads. The conductor region consists of NC number of atoms. Thus, in order to account for some general features of the electronic properties dependence of the system under consideration on the vacancy position, the single vacancy and divacancy are examined in different positions in the device in Fig. 1.

The conductor and the leads are described by tight-binding with one π-electron per atom which is successfully used to study the carbon-related materials. The tight-binding Hamiltonian of the system can be written as:

\[ H = \sum_i \varepsilon_i a_i^\dagger a_i + t \sum_{i,j} a_i^\dagger a_j + \sum_i V a_i^\dagger a_i \]  

where \( \varepsilon_i \) is on-site energy and \( t \) is the hopping matrix element between the nearest neighbours. We only consider the nearest-neighbour interaction. The on-site energies are taken as zero and \( t=2.78 \) eV. The sum in \( i,j \) is restricted to the nearest-neighbour atom, and also \( a_i(a_i^\dagger) \) is annihilation (creation) operator for an electron in the state on site \( i \). A vacancy is simulated by setting the hoppings to zero around the vacant site and its on-site energy equals to a large value or \( V/t \). This has been shown to be equivalent to actual vacancies where bonds are explicitly disconnected. Because of the existence of the magnetic field, a phase \( \phi_{ij} \) is added in the hopping element. In what follows, we show how to calculate the transmission of the system. In the absence of thermal effects and the charging terms, the transmission coefficient for electrons from the left lead to the right lead (left to right lead is ideal) with energy \( E \) is related to Green’s functions using Caroli’s formula which provides high numerical accuracy and efficiency:

\[ T = Tr(\Gamma_m G^r C \Gamma_n G^n) \]  

where \( G^r,a \) are retarded and advanced Green’s functions of the conductor and \( \Gamma_{m,n} \) are coupling matrices from the conductor to the leads. The systems have four leads, resulting in a conductor Green function of form:

\[ G_i = [(E+i\eta)I-Hc-\Sigma'_{m}-\Sigma'_{n} - \Sigma_n]^{-1} \]  

where \( I \) is the identity matrix, \( \Sigma_n \) denotes the self-energy due to the coupling between the conductor and lead \( n \), \( i\eta \) is a small imaginary term added to make the Green’s function (G) non-hermitian. When there are more than two leads, the matrix algebra in Eq. (3) is somewhat more complex as described in the Ref. (23). The coupling matrices are expressed as:
The function $\Gamma_n$ is called the broadening function and describes the coupling of the device to the leads, where $\Sigma_n' = (\Sigma_n')^*$.

The conductor region consists of $N_c$ atoms (where $N_c=32$), making all the matrices $N_c \times N_c$ square matrices. Integrating the transmission probability over the whole energy range and for the external bias applied to the electrodes, one can derive the tunneling current as the form:

$$I(V, E) = 2e / h \left[ T(V, E) \right] [f(E - \mu_n) - f(E - \mu_m)] dE$$

where $T(V, E)$ is transmission probability per channel at the energy $E$, $f(E)$ is Fermi-Dirac distribution, and $V$ is the bias voltage applied to the system and $\mu_n$ ($\mu_m$) is the chemical potential at $n$ ($m$) lead $\mu_n = \mu_m + eV$). The conductance $G(E)$ of the four-terminal graphene can be calculated using the Landauer formula:

$$G = 2e^2 / h \frac{\partial T}{\partial E}$$

In order to describe the effect of the vacancy on the conductance quantitatively, we introduce the decreasing rate of the average conductance, which is:

$$D = \frac{\Delta G}{G_0} = \frac{\int E [G_0(E) - G(E)] dE}{\int E G_0(E) dE}$$

where $G_0(E)$ is the conductance of a four-terminal graphene without vacancy and $G(E)$ is the conductance of the four-terminal graphene with vacancy.

In semiconducting materials, the mean free path $\ell_e$ is very important to assess transport efficiency of the system and the corresponding device performances, indeed $\ell_e$ is a physical length in mesoscopic transport. We note, however, that recent theoretical and experimental work have dealt with ballistic transport in mesoscopic graphene which shows universal behaviour in the regime where $\ell_e > W > L$, where $W$ and $L$ are the sample width and length. Here, elastic mean-free path is extracted numerically from the length scaling analysis of the quantum conductance by considering that, according to the considered regimes,

$$T = N / (1 + L / \ell_e)$$

where $N$ is the number of active conduction channels, $L$ is the length of the central conductor region; $\ell_e$ is the mean free path.

In the present paper, we have calculated all results by ignoring the effects of temperature, spin-orbit interaction, electron-electron correlation, electron-phonon interaction, etc. In this model, it is also assumed that the four side-attached leads have negligible resistance.

### 3 Results and Discussion

Figure 2 shows the transmission coefficient of electrons from lead $L$ to lead $R$ in four-terminal device under the influence of single vacancy. The transmission coefficient through the pure device is shown in Fig. 2 for comparison also. We find that single vacancy affects the band structure and as a result affects the conduction channels and decreases the conduction in comparison with the case that the system is pure. Our results show that a vacancy existing in the four-terminal graphene will deteriorate the electronic conductance in the conduction band region due to destructive interference of electronic waves. Due to the specific electronic structure of graphene, missing one carbon atom creates "vacancy state" at the zero (i.e. Dirac) energy. This vacancy state is quasi-localized and modifies the conduction properties of the device. If we make a single vacancy at a vacant site in a graphene sheet, a vacancy bound state appears at $E = 0$ and its wave function has a non-bonding character, where the amplitudes of the vacant

![Graph showing transmission coefficient](image-url)
sites are zero. The fine peaks in pure curves, known as Van Hove singularities (VHSs), correspond to extreme points in the energy bands and the new peaks in the transmission curve with vacancy correspond to quasi-localized states. The quasi-localized states can be found in the scanning tunneling spectroscopy (STS) images or low bias scanning tunneling microscopy (STM) images. The injected electron will be reflected when its energy is equal to the energy level of the quasi-localized states.

The inset of graph shows the transmission coefficients in the vicinity of the Fermi energy in the presence of two near and far vacancies.

Figure 2 shows the transmission coefficient of electrons from lead L to R in four-terminal graphene nanodevice under the influence of divacancy. It is assumed that inter-vacancy distance \( d \) is small \( (d=a) \), where \( a \) is the distance between two different carbon atoms. The divacancy creates two peaks in the transmission coefficient at energies above and below the Fermi energy. Creating a vacancy in one site is similar to lowering the electronic density of states and increasing the electronic density on all the different sites around the vacancy site. The peaks appearing symmetrically around Fermi energy are due to the bounding and anti-bounding states. In Fig. 3, magnetic field and divacancy are applied to the system simultaneously. The effect of the magnetic field on transmission is two fold: (1) the magnetic field leads to non-dispersive magnetic levels, with a large degeneracy; (2) the energy level spacing is modified giving rise to a piling up of energy levels as one moves away from the Dirac point.

The existence of divacancy along with the magnetic field creates additional band between Landau levels.

The states in the center of the Landau levels are extended and their wave functions are delocalized. Note that our discussion is valid for weak magnetic fields. We find that two close vacancies may couple to each other, forming a “vacancy molecule” tuned by the magnetic field. The coupling between the wave function of two vacancies is verified by determining the distance between them and the magnetic field. If the two single vacancies are introduced far from each other in the lattice, they cannot be coupled each other, then we assume that inter-vacancy distance \( (d=a) \) is small. The bonding between these vacancies can be tuned by magnetic field; this effect is appeared by creating a peak in Fermi energy when the magnetic field and divacancy are applied to the system simultaneously (see the inset of Fig. 3).

In order to investigate the behaviour of changes in current voltage from lead L to lead R, and also investigating the effect of vacancy on current, we apply external potential to the system, so that lead L lies in the potential of \( V/2 \) and lead R lies in the potential of \(-V/2\). The current is not reliable when the applied bias is so big in the mesoscopic system hence the inset of Fig. 4 shows the changes in current voltage in \([-1eV,1eV]\). The small oscillations in the curve are due to Van Hove singularity and originated from the current quantization in this mesoscopic system (see the inset of Fig. 4). It is obvious that the current density increases linearly, at low voltages, and then lowers to a limited value. Decrease of current means that a negative resistance effect appears in
current – voltage characteristics. The reason for this effect is the reduced overlap between the energy band of the two leads (L and R) as the bias is increased. According to the Fig. 4, current in the presence of vacancy in comparison with the pure case, decreases, since the vacancy state produces additional band, in this way the injected electron has more channels for transport and its intensity decreases in comparison with the pure case (by less number of channels). It is obvious that the current increases linearly, at low voltages in the presence of vacancy. Based on Eq. (7), the decreasing rate of the average conductance (between ±0.5 eV) as a function of the central conductor region size ($N_c$) is shown in Fig. 5. The divacancy affects device much more strongly than single vacancy. Moreover, the effect of vacancies decreases when the size of central region increases. This is because there are more atoms in the cross-section of a wider device, so electrons are easier to go around the defect.

To understand conductance scaling in such systems, an analysis of transport length scales is performed. Figure 6, shows the mean free path as a function of the energy $E$ of the injected electrons. Long mean-free paths for electrons near the Fermi energy have indeed been inferred from regular Coulomb oscillations and coherent tunneling at low temperatures\textsuperscript{27,28}. The strong enhancement of $\ell_e$ around the zero energy implies a reduced number of scattering processes. It is well known that scattering of electrons, the charge carriers at graphene device will decrease their mean free path. Here, magnetic field and divacancy are applied to the system simultaneously. In the presence of a magnetic field, the states of graphene are described in terms of Landau levels. At low energies, when the Dirac fermion description is valid, the energy levels are given by:

$$E_n(n) = \pm \sqrt{2\delta l_n^3}$$

and defined $l_n = \sqrt{\hbar/eB}$, $\delta = \frac{3m}{2}$ and $n=1, 2, \ldots$

Notice that the cyclotron energy is much larger than the Zeeman energy, thus, we disregard the Zeeman energy. Both vacancy and the magnetic field can affect the transport properties in the system. There are two important length scales: vacancy causes electron scattering, leading to an electron mean-free path ($\ell_e$) and the magnetic field introduces a magnetic length ($\ell_B$). Electronic states in a Landau level (LL) can be viewed as cyclotron motions of an electron around orbits of radius ($\ell_B$) centered at different location. This should have some consequences on the transport gaps and could be at the origin of large sample-to sample low-temperature conductance fluctuations.

4 Conclusions

Based on Landauer approach and using tight-binding model, the influence of two kinds of vacancy, single vacancy and divacancy in the presence of perpendicular magnetic field on the transport properties of a four-terminal graphene nanodevice, has been studied. Our results show that single vacancy
existing in the four-terminal graphene will deteriorate the electronic conductance in the conduction band region due to destructive interference of electronic waves. We find that divacancy creates bounding and anti-bounding states around Fermi energy due to the increasing electronic density on neighbour sites. In the other hand, existence of two single vacancies with small distance between them, in the presence of magnetic field, produces “vacancy molecules” by coupling between their wave function. From the I-V curve, we found the current quantization in the system, also the current in the system with vacancy decreases in comparison with the pure case, because of the creation of vacancy band. It shows that the effect of vacancies decreases when the size of central region increases. The mean free path patterns are found to strongly depend on the defect. This feature could make such a quasi-2D carbon-based junction a possible candidate for nano-electronic devices.

References