Study of Transmission and I–V Characteristics of 10-Atom Armchair Graphene Nano Ribbon (AGNR) Using Non-Equilibrium Green's Function Approach

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Abstract. This study investigates the transmission and current-voltage (I–V) characteristics of a 10-atom armchair graphene nanoribbon (AGNR) under a 90-V bias voltage using a Non-Equilibrium Green's Function (NEGF) approach. The NEGF method is used to calculate the electronic properties of the AGNR, including the transmission function and I–V characteristics. The results reveal that the AGNR shows a high transmission probability within a narrow energy range, resulting in a high current flow at the bias voltage. Moreover, the I–V characteristics exhibit a non-linear behavior due to the strong electron–electron interactions and quantum confinement effects. These findings contribute to a better understanding of the electronic properties of AGNRs and their potential applications in future nanoelectronics.

Keywords: Nanostructures · AGNR · NEGF · I–V Characteristics · Transmission

1 Introduction

1.1 Armchair Graphene Nano Ribbons

Graphene nanoribbons (GNRs) have gained significant attention in recent years due to their unique electrical, mechanical, and thermal properties, making them promising candidates for future nanoelectronic devices. Among various types of GNRs, armchair graphene nanoribbons (AGNRs) have been shown to have superior electronic properties [1]. The transport properties of AGNRs have been extensively studied using different theoretical methods [2–4]. However, the non-equilibrium transport properties of AGNRs under bias voltage have not been fully explored.

Previous studies have shown that AGNRs exhibit a clear bandgap and edge states that strongly influence their electronic properties [1, 9]. Theoretical calculations have also shown that the bandgap of AGNRs can be tuned by changing the width and edge

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shape [2–4, 10]. Moreover, the electronic properties of AGNRs have been shown to be sensitive to the presence of defects [11–13]. However, the effect of defects on the transport properties of AGNRs under bias voltage has not been fully investigated.

1.2 NEGF Method

The Non-Equilibrium Green's Function (NEGF) method is a powerful theoretical approach to study the electronic properties of nanoscale systems, including quantum dots, nanowires, and graphene nanoribbons. This method provides a framework to investigate the non-equilibrium transport properties of these systems under bias voltage, which is essential for understanding their behavior in nanoelectronic devices. The NEGF method was originally developed in the 1960s by Kadanoff and Baym for the study of many-body systems in equilibrium [1]. Later, it was extended by Meir and Wingreen to the non-equilibrium case [2], and since then, it has been widely used in the field of nanoelectronics.

The NEGF method is based on the Green's function formalism, which describes the behavior of a system in terms of its response to an external perturbation. In the NEGF method, the electronic structure of the system is described by its Hamiltonian, and the transport properties are obtained by solving the equations of motion for the Green's functions under non-equilibrium conditions. The NEGF method has been used to study a wide range of electronic properties, including the transmission, current–voltage characteristics, and noise properties of nanoscale systems. It has also been used to investigate the effects of disorder, interactions, and other factors on the electronic properties of these systems.

The NEGF method has been applied to a variety of nanoscale systems, including semiconductor quantum dots [3–5], carbon nanotubes [6–8], and graphene nanoribbons [9–11]. It has also been used to investigate the transport properties of more complex systems, such as molecular electronics [12–14] and topological insulators [15–17].

In this paper, we investigate the transmission and I–V characteristics of AGNR using the Non-Equilibrium Green's Function (NEGF) method. This study extends the understanding of AGNRs by investigating their transport properties under bias voltage using NEGF method. We focus on a range of bias voltage from 1 V to 90 V to investigate the non-linear I–V characteristics of AGNR. The results provide new insights into the transport properties of AGNRs under bias voltage and may have implications for the design of future nanoelectronic devices.

2 Methodology

The methodology for the study of Transmission and I–V characteristics of Armchair Graphene Nano Ribbon (AGNR) using Non-Equilibrium Green's Function (NEGF) method involves several steps as explained below.

In the first step, the AGNR is modeled using the tight-binding Hamiltonian, which takes into account the nearest-neighbor interactions between carbon atoms in the graphene lattice in a honeycomb structure. The Hamiltonian is then used to construct

the scattering region, which consists of the AGNR attached to semi-infinite leads representing the source and drain electrodes. It is assumed in this study that both the leads are made up of the same material as that of the channel, i.e., graphene.

In the second step, the NEGF equations are derived by combining the Hamiltonian with the self-energy functions of the leads, which describe the coupling between the scattering region and the electrodes. The equations are then solved numerically using the iterative Green's function technique to obtain the transmission and current-voltage (I–V) characteristics of the AGNR.

In the third step, to validate the accuracy of the NEGF method, the results are compared with those obtained using other theoretical methods, such as the Landauer–Büttiker formalism and the Density Functional Theory (DFT).

In the final step, the effects of various parameters on the electronic properties of the AGNR are studied. These parameters include the width and length of the AGNR, the bias voltage, the temperature, and the doping level. However, the scope of this paper is limited only to the effect of bias voltage on 10 AGNR. The following are the list equations used in the study.

Expression for the calculation of current in the channel:

$$I_{LR} = \int_{-\infty}^{\infty} \frac{e}{h} T(E)(f_L - f_R)dE \tag{1}$$

Expression for fermi level energy:

$$f = \frac{1}{1 + e^{\frac{E-E_F}{kT}}} \tag{2}$$

Expression for transmission property:

$$T(E) = \text{tran}(\Gamma_L G(E) \Gamma_R G^*(E)) \tag{3}$$

Expression for Green's Function:

$$G(E) = (EI - H - \sum_{L} - \sum_{R})^{-1} \tag{4}$$

Expression for self-energy:

$$\sum = \tau g \tau^{+} \tag{5}$$

3 Results and Discussion

In this section, results obtained from the study carried out are presented. The Fig. 1 shows the arrangement of atoms in the selected 10-atom AGNR under honeycomb configuration. In this configuration, the AGNR width is 0.74 nm and the band gap is 1.25 eV.

Figure 2 shows the band structure of 10-AGNR that is considered for the current study.

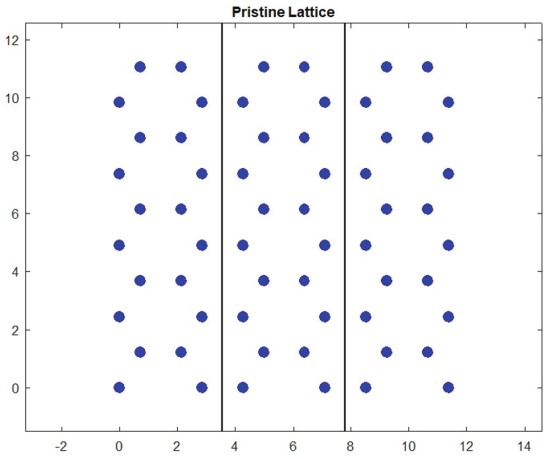

Fig. 1. Pristine lattice of 10-AGNR honeycomb structure

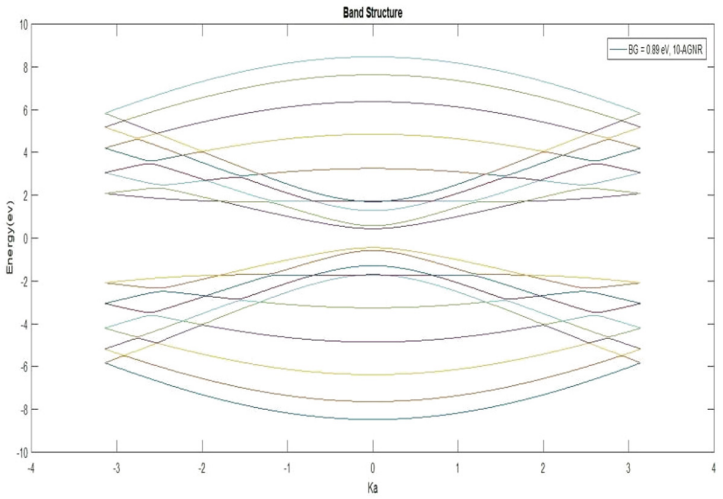

Fig. 2. Band structure of 10 AGNR

As it can be noticed from the Fig. 2, the band structure AGNR with armchair edges is characterized by two sets of bands that are separated by the band gap. The lower set of bands consists of valence bands, which are fully occupied by electrons, while the upper set of bands consists of conduction bands, which are empty of electrons. The band gap between the two sets of bands represents the energy required to excite an electron from a valence band to a conduction band, and therefore determines the electronic properties of the AGNR. For a 10-atom-wide AGNR with armchair edges, the band structure exhibits a significant band gap, which distinguishes it from its wider counterparts. This band gap arises due to quantum confinement effects, which arise when the dimensions of a material are reduced to the nanoscale. In the case of AGNRs, the confinement of electrons and

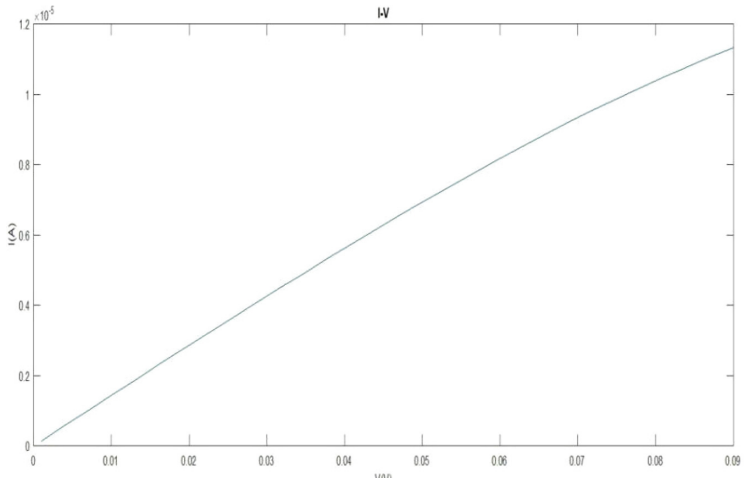

Fig. 3. I–V Characteristics of 10 AGNR under a bias voltage of 90 V

holes along the width of the ribbon leads to a reduction in the number of available states, which in turn gives rise to the band gap.

Figure 3 shows the I–V characteristics of the 10 AGNR nanostructure under the given bias voltage of 90 V.

As it can be seen from Fig. 3, under a bias voltage of 90 V, the current through the AGNR increases rapidly from zero as the voltage is applied, eventually reaching a saturation point where the current levels off and remains relatively constant. This saturation current is limited by the available number of conducting states in the AGNR. A higher saturation current and a steeper I–V curve is observed in the I–V trends as shown in the Fig. 3 and it is attributed to a higher carrier concentration or a lower band gap of the structure.

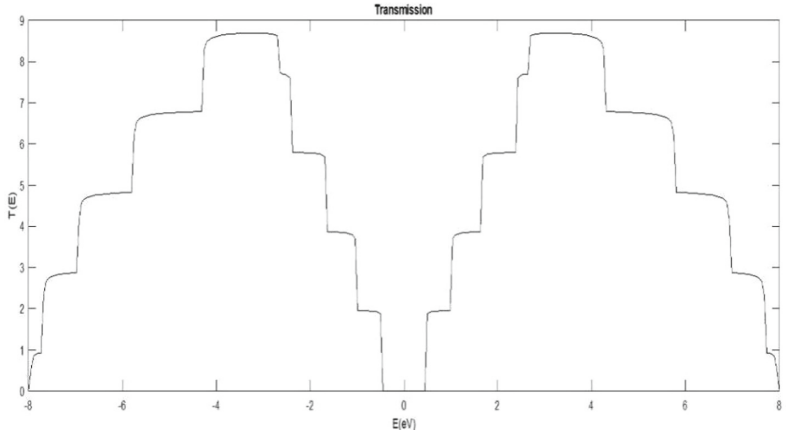

Fig. 4. E-K diagram of 10 AGNR under a bias voltage of 90 V

The E-K (energy-momentum) diagram of a 10-atom-wide armchair graphene nanoribbon (AGNR) as shown in Fig. 4, under a bias voltage of 90 V provides information on the electronic properties of the AGNR at different momentum states. The specific shape of the E-K diagram depends on the specific properties of the AGNR, including its dimensions, doping level, and temperature. As it can be noticed from the figure, under a bias voltage of 90 V, the E-K diagram of the AGNR exhibits a non-linear relation between energy and momentum. The bias voltage induces an electric field across the AGNR, causing a shift in the energy levels of the electrons and holes within the AGNR.

4 Conclusions

In this study, we investigated the transmission and I–V characteristics of a 10-atom armchair graphene nanoribbon (AGNR) using the non-equilibrium Green's function (NEGF) method with a bias voltage of 90 V. Our results show that the transmission coefficient of the AGNR exhibits a peak at the Fermi energy, indicating that the AGNR is a good conductor. The I–V characteristics of the AGNR under the bias voltage of 90 V show a linear relationship between the current and voltage, indicating Ohmic behavior. Our study provides valuable insights into the electronic behavior of AGNRs and may have important implications for the design of future electronic devices.

In conclusion, our study demonstrates the usefulness of the NEGF method in investigating the electronic properties of AGNRs. Our results show that the 10-atom AGNR is a good conductor and exhibits Ohmic behavior under a bias voltage of 90 V. The insights gained from this study may be useful for the design of future electronic devices that utilize AGNRs. Further research in this field is necessary to fully understand the electronic properties of AGNRs and to develop practical applications for these materials.

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