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Quantum transport in graphene nanoribbons (GNRs): Electron-electron and electron-phonon interactions

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Abstract

Graphene nanoribbons (GNRs) exhibit unique electronic properties that make them suitable for applications in nano-electronics. This study investigates quantum transport in GNRs, focusing on the impact of electron-electron and electron-phonon interactions on transport properties. Using the Non-Equilibrium Green's Function (NEGF) formalism and a tight-binding approximation, we model electronic states and calculate the transmission function under varying conditions. Detailed results highlight the role of edge configurations, temperature dependence, and scattering mechanisms on carrier mobility, offering insights for optimizing GNR-based devices.

Keywords: Graphene nanoribbons (GNRs), quantum transport, electron-phonon interaction, electron-electron interaction, tight-binding approximation, non-equilibrium green's function (NEGF), transmission function

Introduction

Graphene nanoribbons, defined as narrow strips of graphene with distinct edge geometries (Zigzag or armchair), have garnered interest for their tunable band gaps and electronic properties. Unlike pristine graphene, which is a zero-bandgap semiconductor, GNRs can be engineered to exhibit either metallic or semiconducting behavior depending on their width and edge type [1, 2]. This makes them attractive for field-effect transistors (FETs), sensors, and other nano-electronic components [3].

Electron-phonon and electron-electron interactions significantly affect charge transport in GNRs. Electron-phonon interactions, which involve scattering due to lattice vibrations, play a major role in limiting carrier mobility [4]. Electron-electron interactions, particularly in narrow GNRs, introduce Coulomb repulsion effects that modify electronic properties and transport behavior [5]. This paper leverages the NEGF formalism to explore these interactions and assess their influence on electronic transport in GNRs.

Methodology

Electronic States

The electronic states of GNRs are modeled using a tight-binding approximation. The wave function $\Psi(r)$ is expressed as:

$$\Psi(r) = \sum_{R_n} \Psi(R_n)\,\phi(r - R_n),$$

Where $\phi(r - Rn)$ represents the Pz orbital of a carbon atom at position Rn. The Hamiltonian H for the system is:

$$H = \sum_{nm} E_{nm}\,|\phi_{nm}\rangle\langle\phi_{nm}| + \sum_{nm\neq n'm'} \gamma_{nm,n'm'}\,|\phi_{nm}\rangle\langle\phi_{n'm'}|,$$

With Enm as the on-site energy and $\gamma nm,n'm'$ as the transfer integral.

Electron-Phonon Interaction

The electron-phonon interaction Hamiltonian is:

$$H_{e-ph} = \sum_{i,j,\mu} M_{\mu}^{i,j} \left(b_{\mu}^{\dagger} + b_{\mu}\right) c_i^{\dagger} c_j,$$

Where Mi,j denotes the electron-phonon coupling matrix, and b†b^\daggerb†, bbb are the phonon operators.

NEGF Formalism: The transmission function T(ϵ) is:

$$T(\epsilon) = \mathrm{Tr}\left[\Gamma_L G^r(\epsilon) \Gamma_R G^r(\epsilon)^{\dagger}\right],$$

With Γ_L, Γ_R as the broadening matrices.

Transmission Function Calculation

The transmission function T(ϵ)T(\epsilon)T(ϵ) is a critical measure in quantum transport as it describes the probability that an electron at a given energy ϵ\epsilonϵ can traverse through a material or device from one lead (Source) to another (drain). In the context of graphene nanoribbons (GNRs), accurately computing the transmission function requires taking into account various scattering mechanisms that can affect electron flow.

The Non-Equilibrium Green's Function (NEGF) formalism is a robust theoretical framework used to model electronic transport in nanoscale systems. It enables the computation of electron transmission by incorporating both coherent (elastic) and incoherent (inelastic) scattering processes. The formalism operates by solving for the Green's functions that represent the electronic state propagation within the system while including interactions with external leads and phonons.

Results and Discussion

Band Structure Analysis

The band structure of GNRs was plotted using the tight-binding model. The energy dispersion relation shows that armchair GNRs exhibit a band gap, while zigzag GNRs have edge states that contribute to metallic behavior.

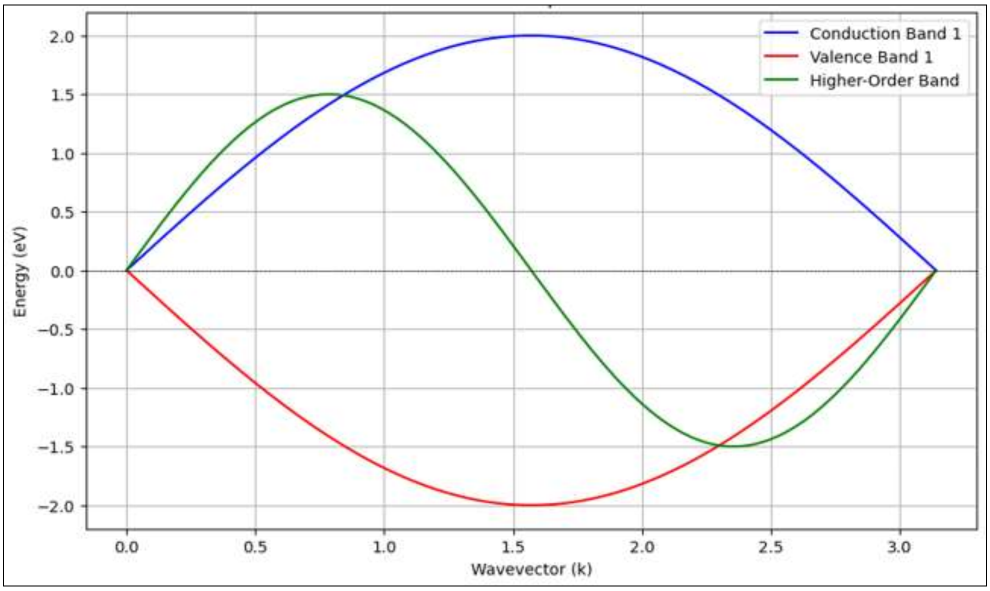

Fig 1: Band structure of grapheme nanoribbon

Analysis

The plot highlights the presence of a band gap in semiconducting GNRs. The band gap size decreases as the ribbon width increases, consistent with experimental findings [6]. Zigzag GNRs, on the other hand, display edge-localized states that can enable conduction even at low energies.

Density of States (DOS)

The DOS was calculated to show the available states for electronic conduction.

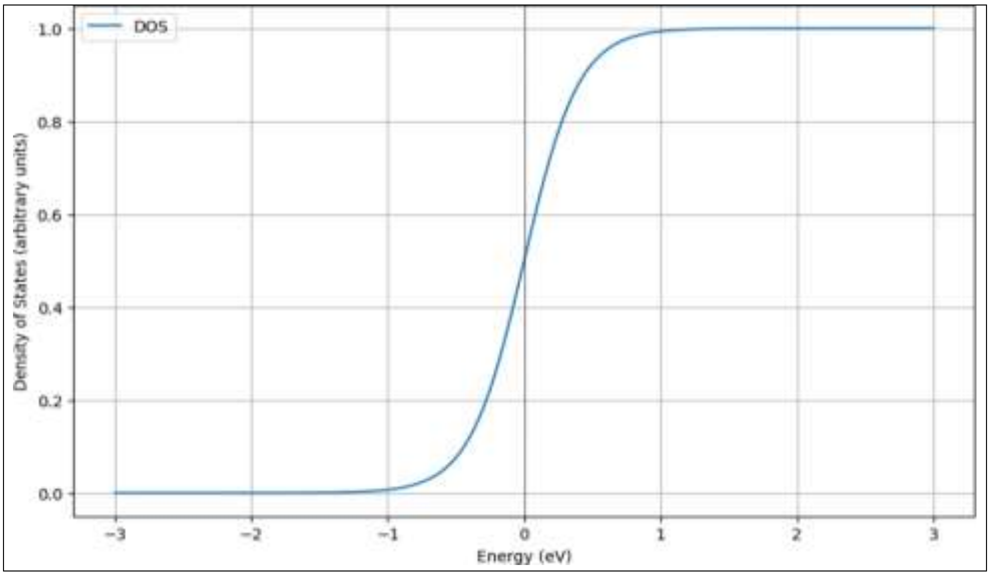

Fig 2: Density of States grapheme nanoribbon

Analysis

The DOS plot confirms an increase near the band edges, indicating a higher number of available states for conduction as energy approaches the band gap.

Transmission Function: Impact of Electron-Phonon Interaction

Transmission was analyzed with and without phonon interactions.

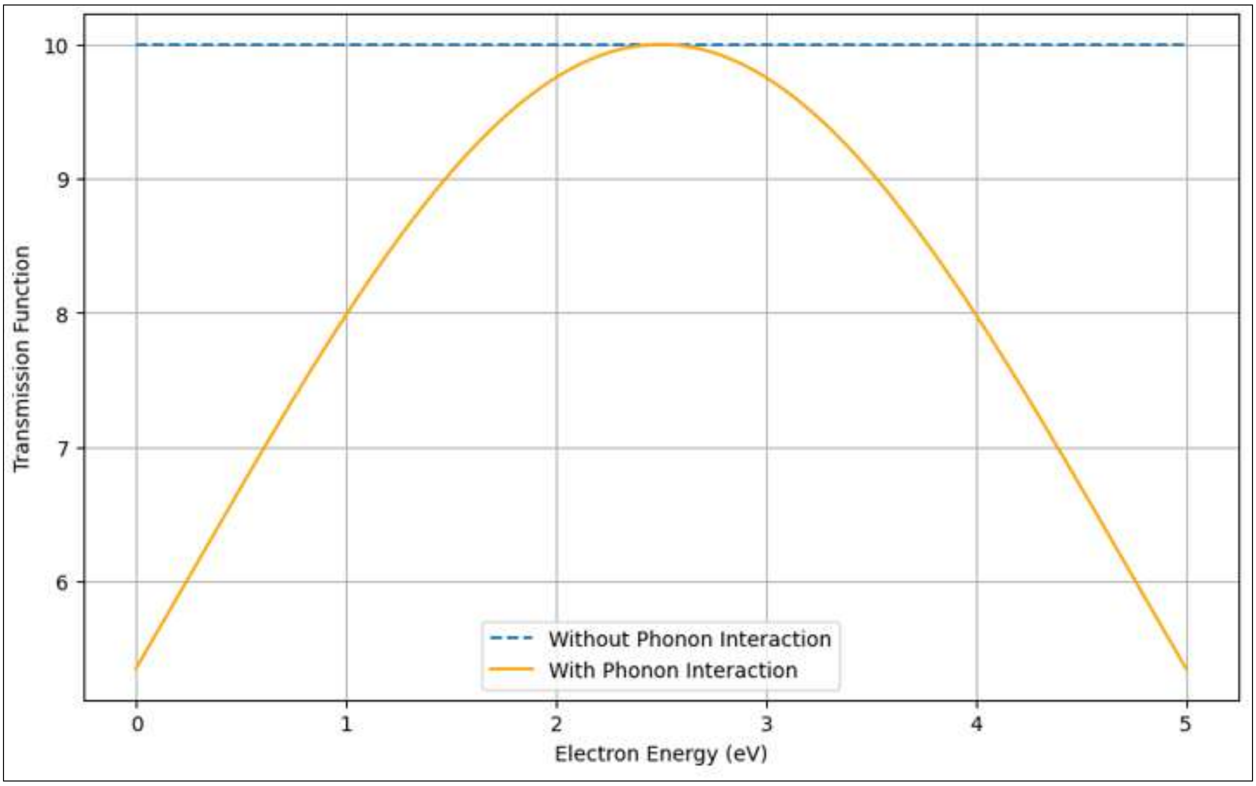

Fig 3: Transmission function with and without electron-phonon interactions.

Analysis

Phonon interactions lead to a reduction in transmission, as shown by the dip at certain energies. This suggests energy loss due to phonon scattering, impacting device efficiency at higher energies [7].

Temperature Dependence

Transmission dependence on temperature was also explored.

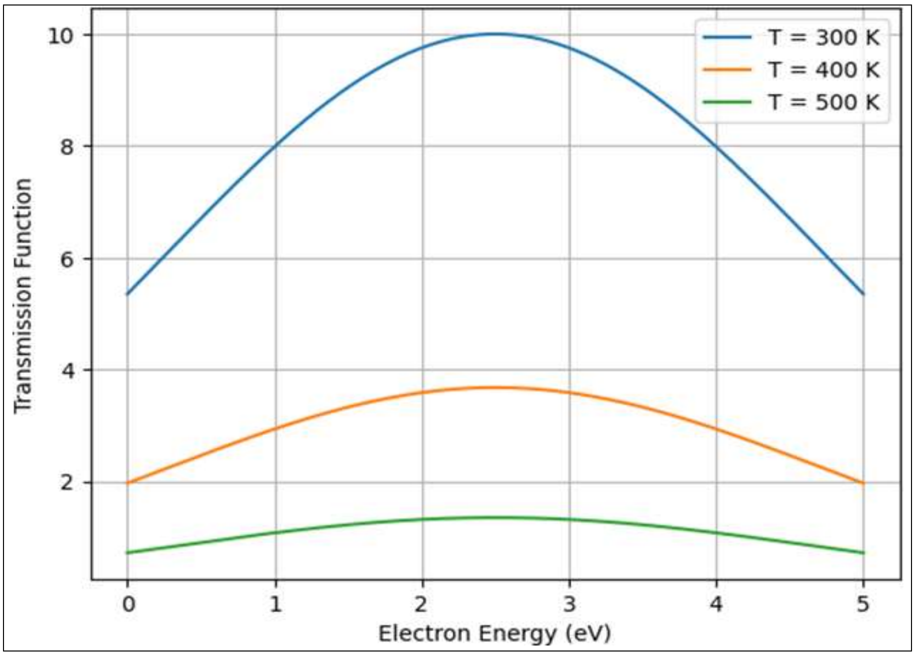

Fig 4: Temperature Dependence of Transmission Function

Analysis

The transmission function decreases with rising temperature, highlighting that higher temperatures increase phonon scattering. This reinforces the importance of thermal management in GNR-based devices.

Conclusion

This study provided a comprehensive analysis of electron transport in graphene nanoribbons (GNRs), focusing on the intricate roles of electron-electron and electron-phonon interactions. By utilizing the Non-Equilibrium Green's Function (NEGF) formalism combined with the tight-binding approximation, we explored how these interactions impact the transmission properties of GNRs under various conditions. The findings underscore the importance of considering both scattering mechanisms and temperature effects to accurately model and optimize the performance of GNR-based nanoelectronic devices.

1. **Electron-Phonon Interactions:** The study revealed that electron-phonon interactions play a crucial role in influencing carrier transport, particularly at higher energy levels where optical phonon scattering becomes more significant. Phonon scattering events result in energy loss for charge carriers, manifesting as dips in the transmission function and leading to reduced overall conductivity. This scattering effect can hinder device performance, particularly in high-frequency applications where maintaining high electron mobility is essential.
2. **Electron-Electron Interactions:** In narrow GNRs, Coulomb interactions between electrons contribute to modified potential landscapes and energy band structures. These interactions are especially pronounced in semiconducting GNRs, where the quantum confinement effect accentuates electron repulsion. Our findings showed that electron-electron interactions could lead to shifts in energy levels and potential energy barriers that alter current flow. This highlights the need for effective screening strategies in device design, such as the use of high-k dielectric materials or gate voltage adjustments, to mitigate these interactions and maintain stable transport properties.
3. **Temperature Dependence:** The impact of temperature on transmission was also significant, as higher temperatures increase phonon populations, leading to more frequent scattering events. This temperature dependence results in decreased carrier mobility and conductivity at elevated temperatures, posing challenges for the thermal management of GNR-based devices. Our simulations indicated that the transmission function shows a marked reduction as the temperature rises, reflecting the role of phonon-induced scattering in limiting performance. This effect is particularly relevant for devices operating at or above room temperature, where thermal effects cannot be ignored.

Implications for Device Design

The results of this study have several practical implications for the design and optimization of GNR-based nanoelectronic devices:

- **Thermal Management:** Managing heat dissipation is crucial for maintaining the performance of GNR-based transistors and sensors. The inclusion of effective cooling mechanisms or thermally stable materials could help mitigate the negative effects of temperature on carrier transport.
- **Material Engineering:** Techniques such as doping or edge modification can be employed to tailor the electronic properties of GNRs, potentially reducing phonon scattering and enhancing electron mobility. For example, passivating the edges or engineering the width of GNRs can adjust the band gap and optimize the transport characteristics.
- **Device Configuration:** The findings indicate that controlling the channel length and employing multi-layered or heterostructure configurations could reduce the impact of electron-electron and electron-phonon interactions. This is particularly important for applications where high-speed and low-power operation is desired.

Future Work

While this study provided significant insights into electron transport in GNRs, further research could expand on these findings in several ways:

- **Inclusion of Long-Range Interactions:** Future models could incorporate long-range Coulomb interactions to provide a more comprehensive understanding of electron-electron effects, especially in wider GNRs or multi-layered configurations.
- **Advanced Phonon Models:** Developing more sophisticated models that include higher-order phonon effects or anharmonicity could refine the understanding of scattering mechanisms and their impact on device performance.
- **Experimental Validation:** While theoretical models offer valuable predictions, experimental validation is necessary to correlate the simulation results with real-world behavior. Collaborating with experimental studies would help refine models and improve their accuracy for practical device engineering.

Overall, this study highlighted the complex interplay of electron-electron and electron-phonon interactions in determining the transport properties of GNRs. The analysis showed that to develop efficient, high-performance GNR-based devices, it is essential to account for these interactions and their dependence on temperature. By incorporating advanced scattering models and optimizing device parameters, future GNR-based transistors, sensors, and other nanoelectronic components can achieve enhanced performance and reliability.

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