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Electronic Properties of Graphene Nanoribbons with Zigzag Armchair Edges

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ABSTRACT We have studied the electronic properties of graphene nanoribbons with zigzag armchair edges. We have calculated the local density of states, the single particle special function, the optical conductivity and the conductance for different geometries. We have also studied the disordered effects. The influence of disorder on the transport behavior of tight binding approach has been accepted. The conductance of edge contacted graphene nanoribbon sensitivity was found dependent on the lead graphene nanoribbon matching conditions. In this respect armchair graphene nanoribbon enabled a somewhat better current injection. Dangling bonds on the graphene nanoribbon side of the interface substantially reduced the conductance. The typical conductance of disordered graphene nanoribbons sandwiched between graphene leads in a junction set up exhibited a negative differential conductivity whenever new transport channels become available by increasing the Fermi level. This accentuates the efficiency of Anderson localization function manifested a precursor of the transition from a current carrying to an Anderson disorder induced insulating behavior which takes place when the size of the disordered active graphene region becomes infinite. The obtained results were found in good agreement with previously obtained results.

KEYWORDS Local Density of State, Optical Conductivity, Conductance, Disorder Effect, Transport Tight Binding Approach, Graphene Nanoribbon, Dangling Bond, Fermi Level.

1. INTRODUCTION

Yuan et al. [1] studied properties of graphene within the Dirac cone approximation, only transitions across the Dirac point that are vertical in momentum space are allowed leading to a frequency independent absorption of undoped graphene. For doped graphene the optical response is greatly reduced for frequencies smaller than twice the absolute value of the Fermi energy due to Pauli's exclusion principle, while for larger frequencies it is roughly given by universal ac conductivity [2]. Breaking through in graphene fabrication and pattering facilitated the realization of graphene based electronics, plasmonics and optics properties. Graphene nanoribbons with varying widths down to a few nanometers and graphene quantum dots have been prepared and operated with field effect transistor, filter polarizer or electronic lens functionalities. The striking electronic properties of these graphene nanoribbon based nanostructures strongly dependent on their geometry and edge shape [3-5]. Graphene nanoribbons with zigzag or armchair shaped edges develop specific band structures [6,7]. Thereby for a realistic modeling of the graphene nanoribbons quasiparticle energies and band gaps, edge passivation, edge closure and edge bond relaxation have to be taken into account [8,9]. In narrow armchair

graphene nanoribbons with hydrogen termination atomic sextets largely affect the band gap and consequently the transport properties [10]. For hydrogen terminated zigzag graphene nanoribbons the spin polarization of edge states comes into play. As a matter of course the enhanced screened coulomb interaction gives rise to significant self energy correlations for both zigzag and armchair graphene nanoribbons [11]. The leads connecting the active graphene element to the electronic reservoirs always play an important role, just as the interfaces in graphene junctions and the substrate. Mucciolo and Lewenkopf [12], studied transport through graphene and graphene nanoribbon based devices are strongly affected by disorder. i.e. screening potentials caused by intrinsic impurities, bulk defects induced by the substrate, ripples, edge roughness, adsorbents atoms at unsaturated dangling bonds at the boundary of the sample and adatom on graphene's open surface. Tikhonenko et al. [13] showed that the chirality of the charge carrier's quantum interference triggered even weak antilocalization. The observations of coulomb diamond like features in device conductance suggested that charge transport in graphene nanoribbons occurs through quantum dots forming along the ribbon due to a disorder potential induced by charged impurities [14]. WeiBe and Fehske [15] used highly efficient Chebyshev expansion. Welle Be et al. [16] used polynomial and Duta [17] used Green function techniques to analyse the electronic properties of graphene nanoribbons with zigzag and armchair edges as well as disordered normal conductor graphene or graphene nanoribbon junctions. We have calculated the local density of states, the optical conductivity and the conductance of different geometries. The influence of disorder on the transport behavior of graphene nanoribbons using tight binding approach was made at a first reasonable starting point [18-21]. Pandey et al. [22] studied ensemble Monte Carlo simulations for band structure in bulk materials, especially in the high field region. All relevant scattering mechanisms including impact ionization were used in the case of zinc sulphide, the use of exchange formalism with a local density approximation band structure for simulations of electron transport has led to modify results for the drift velocity and the average energy. Singh et al. [23] have developed a model for the miniband gap and the related non parabolic dispersions at the limiting of bismuth antimony. They have used an interactive one dimensional two band model and developed an analytical approximation for this model. They have studied band edges and electronic phases as a function of grow the orientation, wire diameter and stoichiometry, including the semimetal phases, the indirect semiconductor phases and the direct semiconductor phases. They have found that bulk materials of bismuth antimony and their alloys have the same symmetry with a rhombohedral lattice structure. The obtained results were compared with previously obtained results.

2. METHOD

The local properties of a graphene sample with broken translational invariance are best reflected by the local density of states

$$\rho_i(E) = \sum_{n=1}^{N} \left|\langle i \,|\, n \rangle\right|^2 \delta(E - E_n)$$

where $|i\rangle = c_i^{\dagger}|0\rangle$ and $|n\rangle$ is a single electron eigen state of H with energy En. The local density of states is directly probed by scanning tunneling microscopy. Theoretically $\rho_i(E)$ be determined to defacto, arbitrary precision by the kernel polynomial method, which is based on the expansion of the rescaled Hamiltonian into a finite series of Chebyshev Polynomials. Exploiting the local distribution approach, the distribution of the local density of states has been used to distinguish localized from extending states, e.g. in order to address the problem of Anderson localization in graphene. In addition to the extraordinary bulk properties of graphene finite graphene structures have very surface states that do not exist in other systems. The spectrum of graphene nanoribbons depends on the nature of their edges: Zigzag or armchair. A zigzag graphene nanoribbon with periodic boundary conditions along the *x*-direction presents a band of zero energy modes. This band is due to surface states living at and close to the graphene edges. The density of states of armchair graphene nanoribbons is gapped at E=0. Zigzag graphene nanoribbons with hydrogen pasivation also have a gapped band structure provided that edge magnetization exists, which is not very likely at least at room temperature. Localized staets also appear of a boundary inside the graphene material exists. The magnetizations show that the internal boundaries are of zigzag and armchair types. The four zigzag boundaries give reason to a band of edge states that show up by a strong peak in the averaged density of states,

$$\rho_{me}(E) = N^{-1} \sum_i \rho_i(E) \text{ at } E = 0.$$

for such graphene nanoribbons with voids the localized states located at the sublattice with open bonds do not allow an analytical solution. To model a rough graphene boundary, we repeatedly remove edge sites carbon atoms with only two nearest neighbors from the graphene nanoribbon, just by setting the corresponding $v_i = \infty$

with probability $p=\frac{1}{2}$. If we create by chance antenna carbon atoms with only one neighbor or isolated atoms, these have been removed as well. Graphene nanoribbon with ideal armchair edges along the *x*-direction, the typical sample depicted was obtained after 30 reiterations. Both the mean density of state and local density of states signal the existence of localized edge states which arise because small zigzag regions are generated at the graphene nanoribbon boundary by the cropping process. The Kernel polynomial method has been used to calculate spectral functions and dynamical correlation functions for disordered graphene nanoribbons. The influence of disorder on the electronic properties of graphene and graphene nanoribbons is of particular in the vicinity of the Dirac point. We have used the short range Anderson disorder

$$V_i \in \left[-\frac{\gamma}{2},\frac{\gamma}{2}\right]$$

and determined the momentum resolved single particle spectral function at zero temperature T=0.

$$A\left(\vec{K},E\right)=\sum_{n=1}^{N}\left|\left\langle n\,|\,\psi\left(\vec{k}\right)\right\rangle\right|^2\delta\left(E-E_n\right)$$

where $\left|\psi\left(\vec{k}\right)\right\rangle=\left(N\right)^{-\frac{1}{2}}\sum_i \exp\left(i\vec{k}\vec{r}_i\right)c_i^{\dagger}|0\rangle\cdot$

where $\left|\psi\left(\vec{k}\right)\right\rangle$ is not a Bloch eigen state of infinite graphene due to its sub lattice structure. The obtained results were compared with previously obtained results.

3. RESULTS AND DISCUSSION

Figure (1) shows the results for $A\left(\vec{k},E\right)$ along paths following Brillouin zone boundary, thereby meeting the Dirac points K and K'. The discreteness of the spectra in the vertical direction is a finite size effect due to small $N_{\underline{a}}$ in graphene nanoribbons with $N=N_{\underline{a}}\times L_{\underline{a}}$ sites, causing a sequence of quasi one dimensional bands with Van Hove singularities. They primarly appeared along the $\overline{K'M'}$. $\overline{KM}$ direction for armchair or zigzag graphene nanoribbons. These finite size signatures have been suppressed by disorder away from the Dirac points but persist near k,k' even for relatively large values of γ as shown in Figure (1)(b), indicating that $E=0$ Dirac fermions are less affected by Anderson disorder. The almost dispersion less band of edge states, appeared in zigzag graphene nanoribbons along $\overline{KM}-\overline{MK'}$ for weak disorder as shown in Figure (1)(c) is destroyed for strong disorder, where only a few localized edge states reside near the K, K' points as shown in Figure (1)(d). The valuable information about the transport properties have been obtained from temperature and filling independent current matrix element density

$$j\left(E_1,E_2\right)=\frac{1}{\Omega}Tr\left[J_x\delta\left(E_1-H\right)\delta\left(E_2-H\right)\right].$$

The trace has been evaluated by a stochastic method using a small number. For graphene, the current matrix element density exhibited finite spectral weight only on an 'x' shaped support in the E_1-E_2 plane. Where the line $E_1=E_2$. E describes the ac optical response due to vertical $\pi-\pi^*$ interband transitions, the line E_1-E_2 accounts for the dc conductivity $\omega=0$. For graphene nanoribbons boundary affected strongly affect these signatures.

Figure (2) shows $j\left(E_1,E_2\right)$ and $\sigma\left(\omega\right)$ for the zigzag case. The spectral signature at $E_1=-E_2$ widens out. Of higher significance there have been additional '+' –shaped absorption feature which has been attributed to optical transitions between edge and bulk state. The optical conductivity at fixed ω according to second line is given by and integral over

$$j\left(E_1=E,\,E_2=E+\omega\right),$$

where the Fermi factors filter out contributions located in the second and fourth quadrant only. They suppress $\sigma(\omega)$ below $\omega = 2[E_F]$, yielding a step feature. If compared to the optical response of bulk graphene, showing besides this step a single maximum at the density of state Van Hove singularity point $\omega = 2t$ only, the edge states in zigzag graphene nanoribbons leaded to a further step at $\omega = [E_F]$ and an additional local maximum at $\omega = t$ is seen in the right panel. For $\omega \to 0$, we have found a Drude peak at $[E_F] > 0$ i.e. at finite filling, whereas $\sigma \to \sigma_0$ at the charge neutrality point $E_F = 0$. We have the study of disordered graphene nanoribbons encased by ordered graphene or metal leads. Defects and impurities are inevitable in graphene based devices.

Anderson disorders with one site potential drawn from a box distribution have been used to model the effects of short range impurity scattering by local imperfections. To characterize the transport through disordered graphene Junctions the conductance was analysed. The obtained results were compared with previously obtained results of theoretical and experimental research works and were found in good agreement.

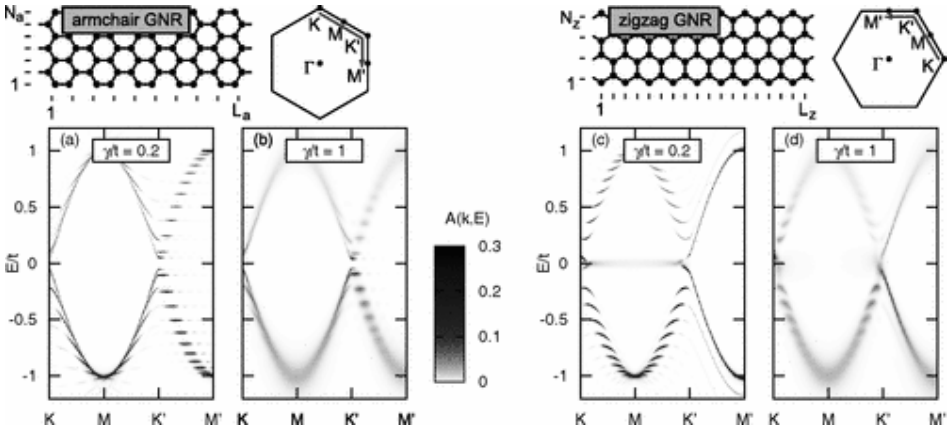

Figure 1: Armchair and zigzag GNRs and orientation of the corresponding Brillouin zine (in longitudinal directions PBC are applied). Bottom panels: Averaged spectral function $A(\vec{k}, E)$ along the red paths indicated in the top panels for Anderson disordered armchair

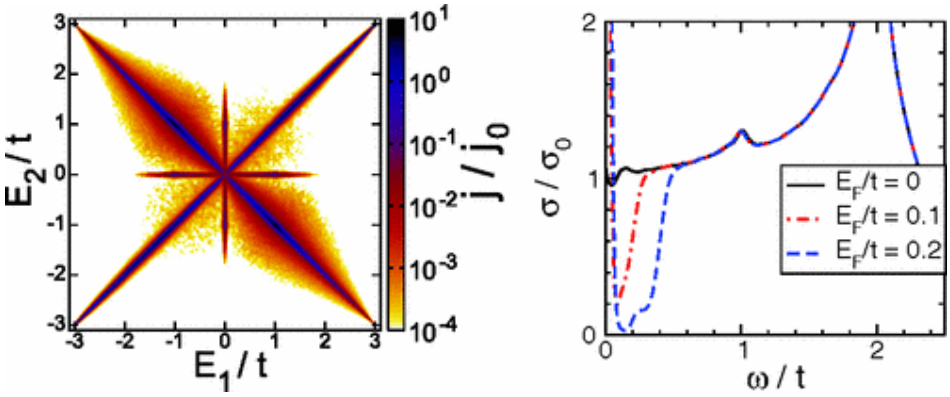

Figure 2: Current matrix-element density $j(E_1, E_2)$ (left panel) and optical conductivity $\sigma(\omega)$ (right panel).

4. CONCLUSION

We have studied the electronic properties of graphene nanoribbons with zigzag armchair edges. Transport through graphene and graphene nanoribbons based devices have strongly affected by disorder, i.e. scattering potentials caused by intrinsic impurities, bulk defects induced by the substrate, ripples, edge roughness, adsorbent atoms at unsaturated daughling at the boundary of the sample and adatoms on graphene's open surface have been found. We have also studied the transport of charge carriers through graphene structures. The kernel polynomial and Green function techniques allowed us to treat actual sized samples beyond the Dirac cone approximation. We have shown that localized edge states dominate the mean density of states of graphene nanoribbons which feature voids or rough surfaces near the charge neutrality point. The sites in the edge region having vanishing amplitude entail a filamentary network of the local density of states in the bulk. For disordered graphene nanoribbons both the averaged single particle spectral function and optical conductivity indicated that disorder tended to suppress the finite size effects caused by the geometry of the nanoribbon. We have found that the contacts and bulk disorder have a major impact on the electronic properties of graphene based devices. In narrow armchair graphene nanoribbons with hydrogen termination automatic sextered largely affected the band gap and consequently transport properties. The couplings have significantly influenced the band gap and hence the transport properties of graphene nanoribbons and Anderson localization owing to bulk disorder. For doped graphene the optical properties is greatly reduced for frequencies smaller than twice the absolute value of the Fermi energy due to Pauli's exclusion principle while for larger frequencies is roughly given by a universal ac conductivity. The efficiency of Anderson localization effected at the band edges of electronically low dimensional systems. For graphene nanoribbon junctions, the conductance distribution function manifested a precursor of transition from a current varying to an Anderson disorder induced insulating behavior which taken place when the size of the disordered active graphene region became infinite. The obtained results are found in good agreement with previously obtained results.

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