

STUDY OF THE GRAPHENE NANORIBBONS WITHIN HUBBARD HAMILTONIAN

N. K. GHOSH

Department of Physics, University of Kalyani, Kalyani-741235, West Bengal, India

e-mail: nanda.ku@rediffmail.com

Received 11 November, 2012

Abstract—Graphene has acquired immense theoretical interest now. The size and geometry of the nanoscale carbon systems have important effects on their electronic properties. In the present work, both the zigzag and armchair grapheme nanoribbons (GNRs) are studied. Simple six sites lattice structure of graphene, made out of interpenetrating triangular lattices, has been considered. Different edge conditions are imposed to model difference in edge geometries. Electron density at the edge-site and in-site have been calculated for both GNRs. With the increase of on-site energy at the edges, the charge density decreases (increases) at the edge-sites (in-sites). The specific heat curves show single-peak structure with almost linear nature at the low temperatures. It confirms that graphene is similar to that of a two level system. The low energy behavior reflects the massless fermion feature of the modes. Observations have been compared with existing results.

Keywords: graphene; nanoribbons; Hubbard Hamiltonian

1. Introduction

Graphene, the two-dimensional flat monolayer of carbon atoms packed into a honeycomb lattice, is of immense experimental [1-3] as well as theoretical [4-6] interest now due to its importance as building blocks for future carbon-based nanoscale electronic devices [7-9]. It is made out of carbon atoms arranged in hexagonal structure. The structure is a triangular lattice with a basis of two atoms per unit cell. The growing interest in graphene is due to its unique properties. It has a high electronic mobility and high charge carrier concentrations [9]. The graphene structure is easily accessible and it is cheap to make. Its many unique properties are still not properly understood and need further investigations.

In [10], authors have investigated the role of edge states in the electronic specific heat and magnetic ordering of graphene strips. Considering Coulomb repulsion U within a mean field approximation, they have obtained the magnetization of the edge sites. They observed that at very low temperatures, the edge states give extra strong enhancement in the specific heat of zigzag strips. The low energy electronic states and heat capacity of graphene strips have been investigated [6]. The Hamiltonian for graphene strips with zigzag and armchair edges has been diagonalized to obtain the density of states. The overall behavior of the heat capacity in graphene is similar to that of a two level system.

Using quantum many-body configuration interaction methods, both zigzag and armchair GNRs have been studied [11] within Hubbard Hamiltonian. They observed that the bipartite nature of the graphene lattice gets destroyed at the edges and the charge density is higher at the edges due to hydrogen passivation of the edge atoms. First principles calculations based on density functional

theory to study quasi one-dimensional edge-passivated (with hydrogen) zigzag graphene nanoribbons reveals that for all doping concentrations the systems stabilize in antiferromagnetic ground states [4].

Specific heat and the magnetic susceptibility of graphene behave differently from the Landau Fermi liquid [12]. A generalized tight-binding model has been proposed for both GNRs and it has been shown that a single tight-binding parameter set accurately reproduce the ab initio transport calculations of GNR based systems [5]. The problem of electron-electron interactions in graphene has been reviewed by Kotov et al. [13]. In the weak coupling regime, they discussed the existence of an emerging Dirac liquid of Lorentz invariant quasiparticles. Formation of strongly correlated electronic states in the strong coupling regime, effects of strong magnetic fields in single layers and some aspects of many-body problem in graphene bilayers have been reviewed. They noticed that topics such as Anderson impurity problem, Kondo effect in bilayers, the problem of magnetism, and superconductivity have not been addressed theoretically and experimentally remaining open for future study.

There exists a gap between model calculation using a Hamiltonian and actual ground state properties of graphene. This has led the theorists to the use of computers searching new directions of computation. Plenty of works has been made in this direction with numerical calculations routinely verifying the analytic results. Inspired by these facts, some investigations have been made on the electronic and thermal properties of graphene strips in armchair and zigzag geometries to enhance our understanding on the graphene system. For this, a six-site basis state has been considered for which exact solution is admissible. The Hubbard Hamiltonian is considered for the GNRs. Low temperature specific heat, electron density at the edge and in-sites are calculated. Observations are compared with few existing results.

2. Formulation

We have used the following Hubbard Hamiltonian for the GNRs

$$H = \sum_{i\sigma} E_i c_{i\sigma}^\dagger c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + t \sum_{\langle i,j \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + H.c.), \quad (1)$$

where the summations extend over all pairs of nearest-neighbors site on a simple two-dimensional square lattice; $c_{i\sigma}$ ($c_{i\sigma}^\dagger$) is the annihilation (creation) operator ($\sigma, \sigma' = \text{spin}$), E_i is the on-site energy, t is the nearest neighbor hopping interaction and U is the on-site Coulomb interaction.

The representative six-site spin state has the form

$$|n_{1\uparrow} n_{1\downarrow} n_{2\uparrow} n_{2\downarrow} n_{3\uparrow} n_{3\downarrow} n_{4\uparrow} n_{4\downarrow} n_{5\uparrow} n_{5\downarrow} n_{6\uparrow} n_{6\downarrow}\rangle, \quad (2)$$

where $\sum_{i\sigma} \langle n_{i\sigma} \rangle = 4.0$. There are altogether 495 basis states. In our exact diagonalization study, the

ground state is taken in the form

$$|\Psi\rangle = \sum_m a_m |\Psi_m\rangle. \quad (3)$$

The coefficients a_m are the solutions of the system of equations

$$M \begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix} = 0, \quad (4)$$

where N is the dimension of the Hilbert space and M is a symmetric matrix with a typical element as

$$M_{mn} = [\langle \Psi_m | H | \Psi_n \rangle - \lambda \delta_{mn}] \quad (5)$$

λ being the lowest solution of the eigenequation

$$\det M = 0 \quad (6)$$

and $|\Psi_m\rangle, |\Psi_n\rangle$ are the basis states. Electron density at the i -th site is given by $\langle n_i \rangle = \sum_{\sigma} c_{i\sigma}^{\dagger} c_{i\sigma}$.

In this paper, low temperature specific heat is calculated using the relation

$$C = k_B \beta^2 \frac{\partial^2}{\partial \beta^2} \ln Z, \quad (7)$$

where $Z = \sum_{\alpha} e^{-\beta E_{\alpha}}$ the sum is taken over all eigenstates, E_{α} 's are the eigenvalues, and $\beta = 1/k_B T$, k_B being the Boltzmann constant (taken as unity).

3. Results and Discussions

Variation of electron density at edge-site with edge-site energies are shown in Fig.1 and Fig.2. Due to unsatisfied valence of carbon atoms at the edges, nonzero negative on-site energy exists at the edges. When hopping interaction is not large ($t < -2.25$), it is observed that electron density at the edge-site is high for both GNRs for edge-site energy = -2.0 , consistent with the results of Dutta et al. [11]. But, for $t = -2.25$, in-site electron density is higher. Accumulation of charges at the edge-sites has also been confirmed by scanning tunneling microscopy images [14]. Charge density decreases with the increase of NN hopping strength t (which increases mobility of electrons to NN-sites). For zigzag GNRs, density at edge site decreases discontinuously with the energy of the edge-site, whereas it is continuous for armchair GNRs.

Fig.3 and Fig.4 show the behavior of electron density at in-site with the edge-site energy. For both the GNRs, electron density at in-site is low compared to that at edge-site [11], and increases with NN hopping strength t . We see discontinuous increase of electron density at in-site with the edge-site energy for zigzag GNRs, but it increases continuously for arm-chair GNRs.

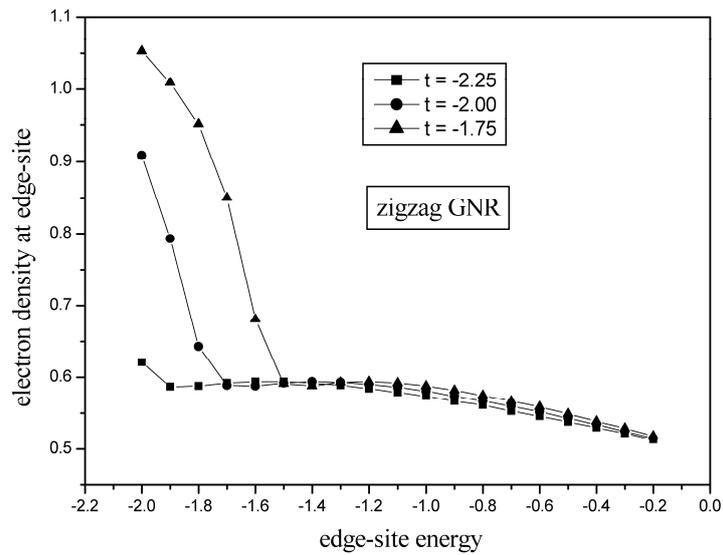


Fig.1. Variation of electron density at edge-site with edge-site energy taking $U = 9.5$.

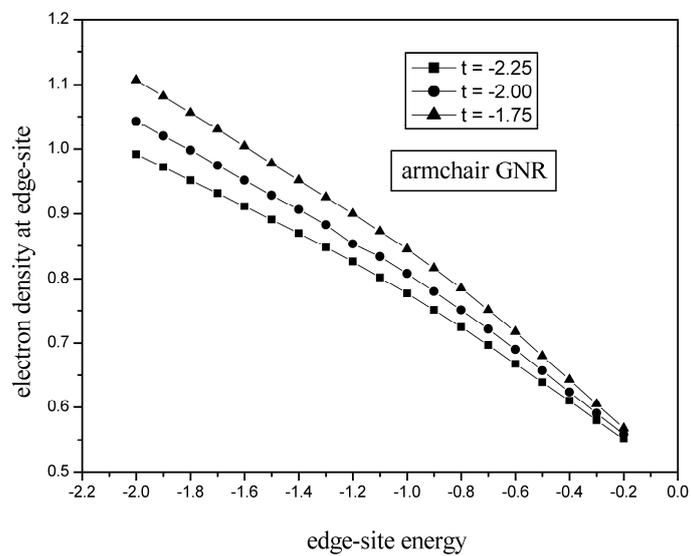


Fig.2. Variation of electron density at edge-site with edge-site energy taking $U = 9.5$.

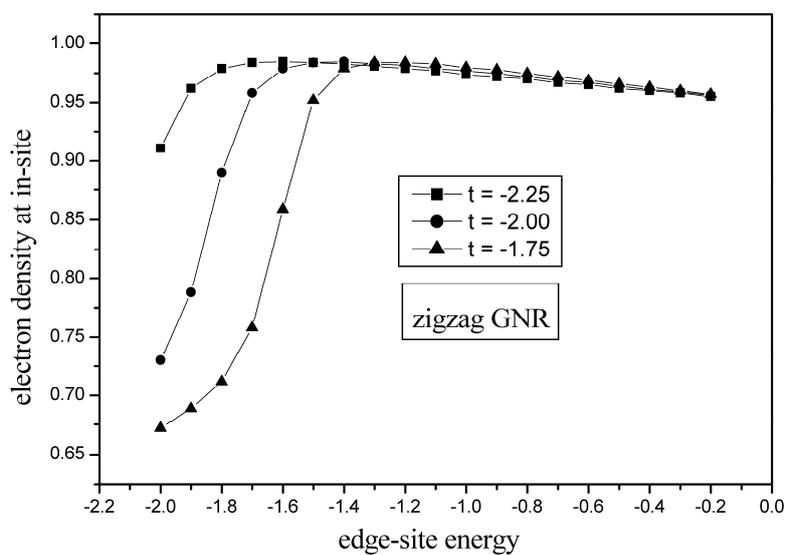


Fig.3. Variation of electron density at in-site with edge-site energy taking $U = 9.5$.

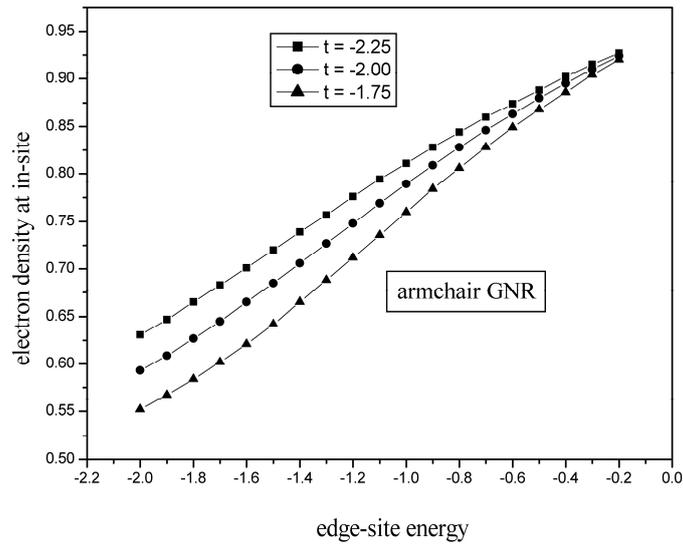


Fig.4. Variation of electron density at in-site with edge-site energy taking $U = 9.5$.

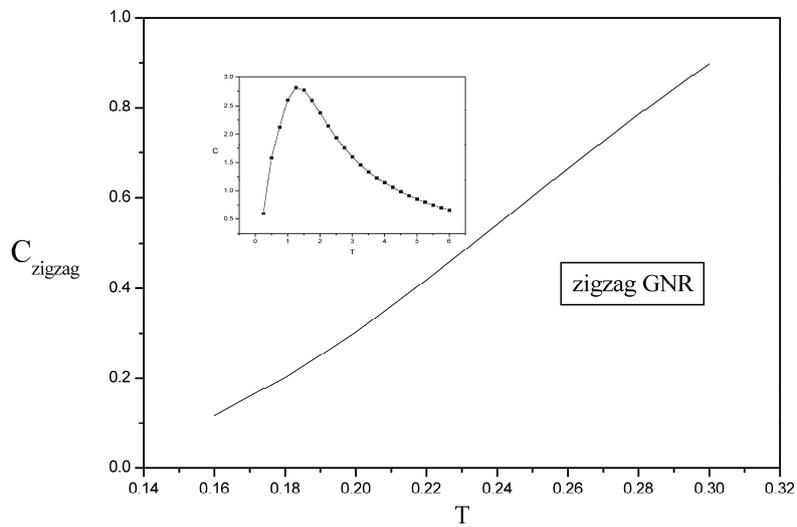


Fig.5. Low temperature specific heat of zigzag GNR taking edge-site energy = -0.2 , $t = -2.0$, $U = 9.5$. Inset shows an overall temperature dependence of C in zigzag configuration.

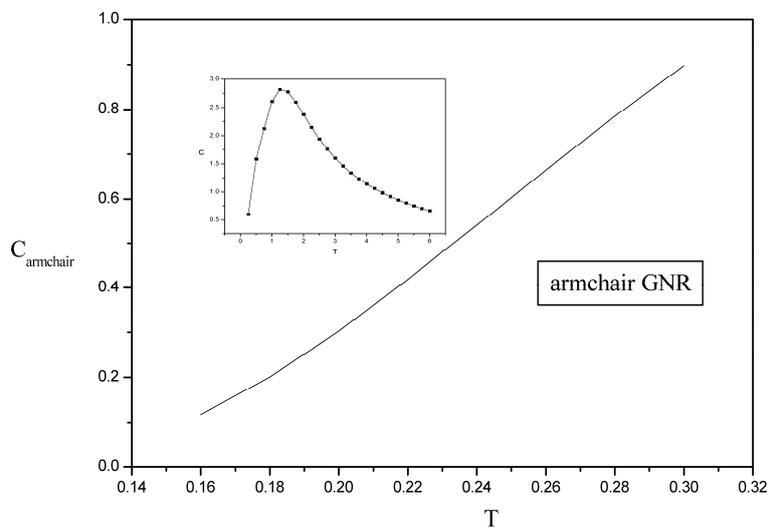


Fig.6. Low temperature specific heat of armchair GNR taking edge-site energy = -0.2 , $t = -2.0$, $U = 9.5$. Inset shows an overall temperature dependence of C in zigzag configuration.

Fig.5 and Fig.6 show the low-temperature behavior as well as overall temperature dependence of electronic specific heat $C(T)$ for both zigzag and armchair GNRs respectively. At very low temperature, specific heat follows a power law behavior: $C = \alpha T + \beta T^2$, where $\alpha = 2.677$ and $\beta = 5.907$. This clearly shows the massless fermion feature of the modes in a graphene strip (for massless fermions in 2D, $C \propto T^2$). The overall variation of C has a single peak which resembles a two-level system. It is observed that $C(T)$ attains a maximum and then decreases as T^{-2} with the increase of temperature. These observations are very much consistent with Yi and Kim [6].

4. Conclusion

Electronic specific heat $C(T)$ and electron densities at edge-site and in-site of different GNRs have been studied using exact diagonalization method. Low temperature behavior of $C(T)$ shows a power law whereas overall behavior predicts a two-level system. For both GNRs, electron densities at edge-site are higher than that at in-site when hopping is not too large. At edge-site (in-site), electron density decreases (increases) with NN hopping strength t . The variation of electron density of zigzag (armchair) GNRs is discontinuous (continuous) with the energy at the edge-sites.

Acknowledgment

Author is thankful to University of Kalyani for financial help.

REFERENCES

1. K.S.Novoselov, A.K.Geim, S.V.Morozov, D.Jiang, Y.Zhang, S.V.Dubonos, I.V.Grigorieva, A.A.Firsov, *Science*, **306**, 666 (2004).
2. A.K.Geim, K.S.Novoselov, *Nat. Mater.*, **6**, 183 (2007).
3. L.Vitali, M.Burghard, P.Wahl, M.A.Schneider, K.Kern, *Phys. Rev. Lett.*, **96**, 086804 (2006).
4. S.Dutta, A.K.Manna, S.K.Pati, *Phys. Rev. Lett.*, **102**, 096601 (2009).
5. Y.Hancock, A.Uppstu, K.Saloriutta, A.Harju, M.J.Puska, *Phys. Rev. B*, **81**, 245402 (2010).
6. K.S.Yi, D.Kim, K.S.Park, *Phys. Rev. B*, **76**, 115410 (2007).
7. G.Dresselhaus, M.S.Dresselhaus, P.C.Eklund, *Science of Fullerenes and Carbon Nanotubes: Their Properties and Applications* New York, Academic Press, 1996.
8. L.Chico, V.H.Crespi, L.X.Benedict, S.G.Louie, M.L.Cohen, *Phys. Rev. Lett.*, **76**, 971 (1996).
9. K.S.Novoselov, A.K.Geim, S.V.Morozov, D.Jiang, M.I.Katsnelson, I.V.Grigorieva, S. V. Dubonos, A.A.Firsov, *Nature (London)*, **438**, 197 (2005).
10. K.S.Yi, D.Kim, K.S.Park, J.J.Quinn, *Physica E*, **40**, 1715 (2008).
11. S.Dutta, S.Lakshmi, S.K.Pati, *Phys. Rev. B*, **77**, 073412 (2008).
12. H.Pei-Song, O.Sung-Jin, Ch.Yu, T.Guang-Shan, *Commun. Theor. Phys*, **54**, 897 (2010).
13. V.N.Kotov, B.Uchoa, V.M.Pereira, F.Guinea, A.H.Castro Neto, *Rev. Mod. Phys*, **84**, 1067 (2012).
14. Y.Kobayashi, K.I.Fukui, T.Enoki, K.Kusakabe, *Phys. Rev. B*, **73**, 125415 (2006).