

Magnetic Nanostructure for Zigzag Graphene Nanoribbons and Application in Nano Electronics

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ABSTRACT

We have studied graphene zigzag edge terminated nanostructures for the magnetic phase diagram considering mean field analysis. In this case four fermion interaction was treated in the magnetic channel. The quantum fluctuations were not captured at the mean field. We have made variational Monte Carlo calculations of the ground state. It was found that the ground state at zero doping was the antiferromagnetic configuration. The edge moment was found smaller than the mean field value due to quantum fluctuations both the antiferromagnetism and ferromagnetism edge moments were stable and they remained unchanged upon increasing the length of the ribbon producing the magnetism robust. The possible chemical modification of graphene nanoribbons to produce and internal doping to engendered the magnetic transition. A ferromagnetic structure of a zigzag edge terminated nanoribbon with boron atom substituted in place of carbons while undoped nanoribbons had a antiferromagnetic configuration within the same calculation. It was found that a Weber Fechner response of nanoribbons played a central role in determining their magnetism. We have formulated a effective theory which led to a magnetic phase diagram of lightly doped nanoribbons including analytical expressions for the width dependence of magnetization, excitation gap and the critical doping needed to engender magnetic transitions. The results found were in good agreement with previously obtained results.

KEYWORDS

Graphene Nanoribbon, Magnetic Phase Diagram, Mean Field Theory, Fermion Interaction, Monte Carlo Simulation, Ferromagnetism, Antiferromagnetism, Excitation Gap.

How to cite this article: Ranjan P. and Chaudhary B.D. (2024). Magnetic Nanostructure for Zigzag Graphene Nanoribbons and Application in Nano Electronics. *Bulletin of Pure and Applied Sciences- Physics*, 43D (1), 25-30.

INTRODUCTION

Neto et al. [1], Nakada et al. [2] and Wakabayashi et al. [3] presented that magnetic moments in zigzag edge terminated honey comb nanostructures was attributed to the edge states. Brey et al. [4-5] and Zarea et al. [6] showed that localized states at the edge were absent into bulk. Ryu and Hatsugai [7] presented that these states were topological origin and was observed using scanning tunneling microscopy [8-9]. Atl and Simons [10] showed that edge magnetism was attributed to the stoner mechanism and was explained through a Landau theory. Some investigators [11-16] studied that the activity in magnetic nanostructures have been driven by their application in nanoelectronics with graphene systems grabbing a significant fraction. Kotov et al. [17] presented that electron interaction and correlations effect on the honey comb lattice contained the phenomena including magnetism [18] and superconductivity [19]. Son et al. [20-21] studied that magnetism at the zigzag terminated edges of graphene by first principle calculations and by a simplified effective Hubbard model [22-28] described by a hopping parameters and site local repulsion. Zhan et al. [29] and Yazyev et al. [30] studied the defect induced magnetism and magnetism of other nanostructures [31]. Bhowmick et al. [32] studied that a zigzag edge terminated nanoribbon produced highly nonlinear response taking to that of sensory organ like eyes and ears. Their density response depended logarithmically on the magnitude of and edge potential applied at the zigzag edges. Bloch et al. [33] showed that Weber Fechner response of these nanoribbons played a central role in determining their magnetism. Karakachian et al. [34], Palacio et al. [35], Wang et al, [36] and Li et al. [37] showed that the tuning the electronic structure of graphene by edge free quantum confinement was found. Ahn et al. [38], Wiesner et al. [39] and Zhang et al. [40] presented that the controlling of geometric structure of graphene and other two dimensional material for strain engineering. Dbrik et al. [41] studied the extra ordinary strong plasmonic behavior of graphene was found as a consequence of the lateral confinement in the arrays of graphene nano corrugation. Guk Ahn et al. [42] performed

density functional theory calculations to study the graphene nano like interaction between the graphene and the substrate played a crucial role in leading to quantum confinement. The longitudinal direction and the effective confined length was found as key parameters to control the electronic structure of graphene by corrugation engineering.

METHOD

The Hamiltonian was used to describe energetic of interacting electron in the honey comb lattice in the Hubbard model as

$$H = -t \sum_{(i,j),\sigma} C_{i\sigma}^\dagger C_{j\sigma} + U e_0 \sum n_{i\uparrow} n_{i\downarrow} - \mu \sum_i n_{i\sigma}$$

Where $C_{i\sigma}^\dagger$ is the operator that creates an electron of spin σ at site i , $n_{i\sigma} = C_{i\sigma}^\dagger C_{i\sigma}$ is the number operator, t is the nearest neighbor hopping amplitude, $U e_0$ is the onsite Hubbard repulsion, $e_0 = \frac{\sqrt{3}}{2} t$ is the characteristic energy scale, U is dimensionless, and μ is the chemical potential. The triangular Bavais lattice has a lattice parameter a , W is the width of the zigzag edge terminated nanoribbon. The Stoner-Landau theory was used for the study. A first order magnetic transition from an antiparallel orientation of the moments on the opposite edges to a parallel orientation upon doping with holes and electrons were considered. For calculations of results the variational Monte Carlo simulations were used. The magnetic phase diagram for generic to zigzag edge terminated nanostructure as nano dots were utilized. Variational quantum Monte Carlo simulations for calculations for results regarding fluctuations was studied considering mean field level. The details of the fully unrestricted numerical mean field calculation of the magnetic phase diagram motivated the analytical theory for development was made. Four fermion interaction term was treated in the magnetic channel. The site dependent quantities were determined by enforcing the self consistency

conditions of mean field theory. The continuum theory which described the low energy of Hamiltonian was taken into account. The this purpose the following relation was used

$$S[\psi] = \int d^{2+1}r \sum_{\sigma} \psi_{\sigma}^*(r) (11\delta_r + H_K) \psi_{\sigma}(r) + Ue_0a^2 \int d^{2+1}r \left[\frac{1}{4}n(r)^2 - \{s^z(r)\}^2 \right]$$

Where $r = (r, \tau)$, $r \equiv (x, y)$ is the position vector, where x coordinate is along the length of the ribbon and y is along the width, τ is the imaginary time and runs form O to β ,

$\psi_{\sigma}^* = (\psi_{A+\sigma}^* \psi_{B+\sigma}^* \psi_{A-\sigma}^* \psi_{B-\sigma}^*)$ is the array of

Grassmann field with $\frac{A}{B}$, sublattice and valley

indices, $n(r) = \sum_{au\sigma} \psi_{au\sigma}^* \cdot \psi_{au\sigma}(r)$ and is the number density,

$S^z(r) = \frac{1}{2} \sum_{av\sigma} \sigma \psi_{av\sigma}^*(r) \psi_{av\sigma}(r)$ is the spin density, 11 is the 4x4 matrix and

$$H_K = v_F \begin{pmatrix} \tau \cdot p & 0 \\ 0 & -\tau^* p \end{pmatrix} = \mu_{11}.$$

Where $v_F = e_0a$ and $p = -i\nabla$, the momentum operator, $\tau = \tau_x e_x + \tau_y e_y$, $\tau_{x,y}$ are Pauli matrixes in the sublattice space, $e_{x,y}$ are the spatial basis vectors. The first order transition from the antiferromagnetism to the ferromagnetism was obtained at a critical doping using the relation.

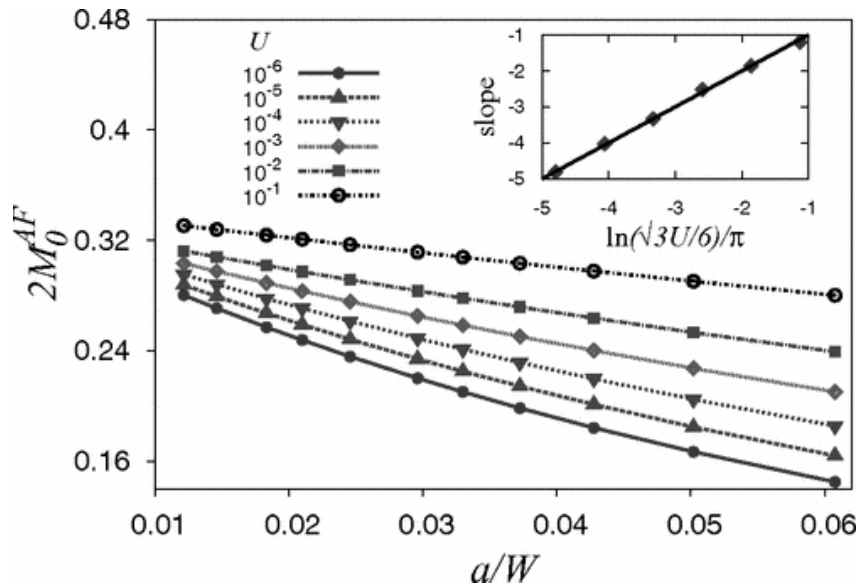
$$\delta_c = C(U) \frac{a}{w}, \quad C(U) = \frac{1 - \sqrt{1 - \ln 3 \left\{ 1 + \frac{2}{\ln\left(\frac{U}{6}\right)} \right\}}}{\pi \left[1 + \frac{2}{\ln\left(\frac{U}{6}\right)} \right]}$$

RESULTS AND DISCUSSION

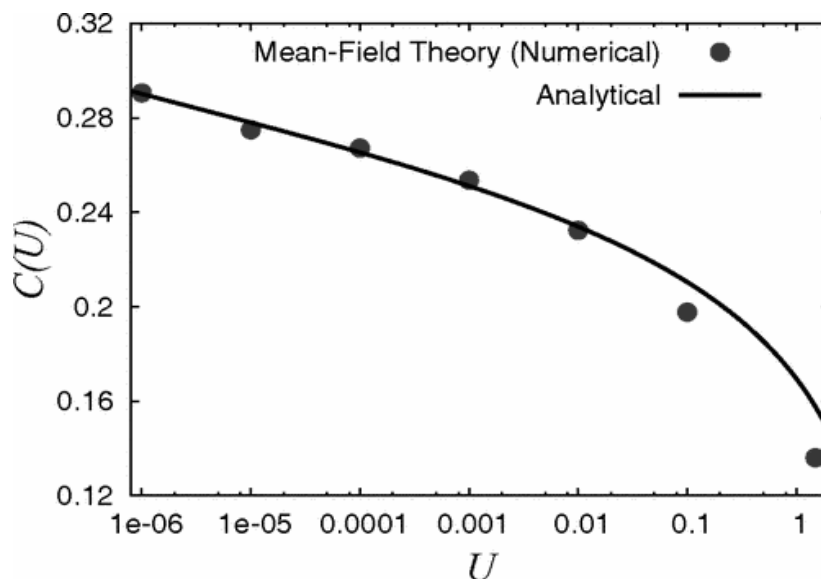
We have studied analytically of the phase diagram for zigzag edge terminated nanoribbons using Hubbard model. A first order magnetic transition from an antiparallel orientation of the moments on opposite edges to a parallel orientation produced upon doping with holes or electrons. The critical doping for the transition was dependent inversely on the width of the ribbon. By applying variational Monte Carlo simulations it was presented that magnetism was robust to fluctuations. It was found that magnetic phase diagram was generic to zigzag terminated nanostructures as nano dots. Graph (1) shows the plot of width dependence of magnetic moment of antiferromagnetism for different values of local site repulsion. It shows a comparison of the analytical results for the antiferromagnetism configuration with the full numerical calculations for undoped nanoribbons. We have found that quantitative agreement of the numerical edge moment with the theory over several site local repulsion were presented. The agreement was also found for the energy gap and for the moment of the ferromagnetism state. It was predicted that the antiferromagnetism was the ground state of the undoped ribbons for any width because spontaneous magnetization of antiferromagnetism was larger than spontaneous magnetization of ferromagnetic. The ground state of the undoped system was always the antiferromagnetism state due to sensory-organ like response of nanoribbons. For doping the system with holes or electron the edge magnetization changed. Graph (2) shows a comparison of the analytical results with

numerical values critical site local repulsion and quantitative agreement was found over interaction parameter. For large values of interaction parameter for graphene the agreement was 10%. This was due to the larger values of interaction parameter resulted in a small contribution from the bulk states. We have made Monte Carlo calculations of the ground state. The Fermi state constructed by imposing an edge magnetization on the edge layers was found. For the antiferromagnetised state the magnetic order parameter was opposite on the two edges while for the ferromagnetised state the magnetic order parameter was equal on both edges. The optimal values of density of state and magnetic order parameter were obtained so as to minimize the ground state energy. We have

found that the ground state a zero doping was the antiferromagnetism with an edge moment 0.20 which was smaller than mean field value 0.27 due to quantum fluctuation. The density response depended logarithmically on the magnitude of an edge potential applied at the zigzag edges. A Weber Fechner response of nanoribbons played a central role in determining their momentum. Due to the calculations of results we have generated a effective theory which led to a magnetic phase diagram of highly doped nanoribbons. The results found were compared with previously obtained results of theoretical and experimental research works and were found in good agreement.



Graph 1: Plot of width dependence of magnetic moment of anti ferromagnetism for different values of local site repulsion.



Graph 2: Plot of dependence of critical site local repulsion on interaction parameter.

CONCLUSION

We have studied magnetic nanostructure for zigzag graphene nanoribbons and their applications in nanoelectronics. An analytical effective theory of the magnetic phase diagram for zigzag edge terminated nanoribbons having Hubbard model with interaction parameter was utilized for the study. It was found that magnetic moment varied with width of the nanoribbon. The magnetic moment in zigzag edge terminated nanostructures attributed to the edge states and localized states at the edge which were exponentially to the bulk and were observed using scanning tunneling microscopy. Edge magnetism was attributed to the Stoner mechanism and were described through Landau theory. The first order magnetic transition from a antiparallel orientation of the moments on opposite edges to a parallel orientation occurred upon doping on holes or electrons. The critical doping for the transition was found to depend inversely on the width of the nanoribbon. The results found were in good agreement with previously obtained results.

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