Orissa Journal of Physics
ISSN 0974-8202

Vol. 23, No.2
August 2016
pp. 141-146

Microscopic Theoretical study of Anti-ferromagnetic order in AA-stacked Bilayer Graphene

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Received: 2.6.2016 ; *Revised : 1.7.2016* ; *Accepted : 1.8.2016*

Abstract. We address here the anti-ferromagnetic (AFM) order present in AA-stacked bilayer graphene in a transverse applied electric field. The system is described by kinetic energy with nearest neighbor electron-hopping with same hopping integral t_1 for both the layers. Besides this the Coulomb interaction exists at A and B sub-lattices with same Coulomb correlation energy. The electron Green's functions are calculated by Zubarev's Green's function technique. The temperature dependent AFM magnetization is calculated from the Green's functions and is computed numerically and self-consistently. The evolution of the AFM magnetization is studied by varying transverse electric field, Coulomb energy and temperature.

Keywords. Coulomb potential , AFM-magnetization, AA- stacked bilayer graphene

PACS No. : 73.22.Pr, 73.22.Gk, 73.21.Ac

1. Introduction

Graphene is a zero band gap semiconductor with unusual properties [1-3]. Recently bilayer graphene becomes a subject of numerous studies to produce graphene based materials with an electronic gap. More over bilayer graphene is an important material itself. More effort has been focused on the study of AB-stacked bilayer graphene [4] than AA-stacked bilayer graphene (AA-BLG) because of availability of good samples [5, 6]. More recently experimental realization of AA-stacked and AB-stacked bilayer (AB-BLG) has been reported [7, 8]. We know that AA-BLG tight-binding spectrum has four bands of which two are electron bands and two are hole bands. The structure of both bands are different in AA-BLG and AB-BLG, In doped AB-BLG, the two bands (one hole band and one electron) touch each other at Fermi point and low energy band

dispersion is nearly parabolic [9,10,11] .The low energy dispersion in AA-BLG is linear similar to mono-layer graphene. The AA-BLG has Fermi surface instead of Fermi points. The important feature of AA-BLG is that the electron and hole surfaces coincide in the undoped material [12]. These degenerate Fermi surfaces are unstable, when an arbitrary weak electron interaction is present and bilayer system becomes an anti-ferromagnetic (AFM) insulators with a finite gap. This electronic instability is strongest, when the bands cross at the Fermi level. The on-site Coulomb repulsion is strongest interaction in AA-BLG system and this interaction is sufficient for stability or meta- stability of the AFM order. The propose of this paper is to investigate the influence of a transverse electric field on the properties of AA-BLG. The degree of suppression of AFM order heavily depends on the effective values of the repulsive impurity potential for hole doping. The tight-binding model Hamiltonian is described in section 2 and the calculation of AFM magnetization is worked out in section 3. The results and discussion are given in section 4 and finally conclusion in section 5.

2. A Tight-Binding Model Hamiltonian

The AA-stacked bilayer graphene consists of two graphene layers having up and down spins. Here each carbon atom of upper layer is placed above the corresponding atom of the lower layer. Each layer consists of two triangular sub lattices A and B. The unit cell of AA-BLG contains four carbon atoms $\mathbf{A_1}$, $\mathbf{B_1}$, $\mathbf{A_2}$ and $\mathbf{B_2}$. Hence the single particle Hamiltonian for AA-BLG is given by

$$H_1 = \sum_{\alpha,k,\sigma} \left(\mu + x\,U_0 - (-1)^{\alpha}\left(\frac{V}{2} + \Delta_A\right)\right) a^{\dagger}_{\alpha,k,\sigma}\; a_{\alpha,k,\sigma} + \sum_{\alpha,k,\sigma} \left(\mu - (-1)^{\alpha}\left(\frac{V}{2} - \Delta_A\right)\right) b^{\dagger}_{\alpha,k,\sigma}\, b_{\alpha,k,\sigma} \qquad (1)$$

Here the Hamiltonian H_1 contains chemical potential μ, impurity concentration x having impurity potential U_0 at A site only in both the layers. V is the applied voltage is perpendicular to the layers with $V \ll t_1$ which corresponds to typical experimental conditions [13,14]. The AFM gap (Δ_A) which is produced due to difference of electron concentrations of opposite spins in both the sub-lattices in the two layers of AA-BLG. Here $a^{\dagger}_{\alpha,k,\sigma}$ and $a_{\alpha,k,\sigma}$ ($b^{\dagger}_{\alpha,k,\sigma}$ and $b_{\alpha,k,\sigma}$) are the creation and annihilation operators of electrons with spin σ in the layers $\alpha = 1, 2$ on the sub-lattices $A(B)$. The Hamiltonian for first-nearest neighbor hopping of electrons and interlayer hopping is given by

$$H_2 = \sum_{<\alpha,k,\sigma>}(\epsilon_k\, a^{\dagger}_{\alpha,k,\sigma}\, b_{\alpha,k,\sigma} + \epsilon^{*}_{k}\, b^{\dagger}_{\alpha,k,\sigma} a_{\alpha,k,\sigma}) \quad (2)$$

$$H_{AA} = \sum_{\alpha,\beta,k,\sigma} [\, \epsilon_{k,\perp} a^{\dagger}_{\alpha,k,\sigma} a_{\beta,k,\sigma} + \epsilon^{*}_{k,\perp}\; b^{\dagger}_{\alpha,k,\sigma} b_{\beta,k,\sigma} + h.c.\,]$$

$$\alpha, \beta = 1\,, 2\;\; \&\;\; \alpha \neq \beta \quad (3)$$

The Hamiltonian H_2 in equation (2) represents the hopping of electrons to nearest-neighbor lattice points having hopping energy $\epsilon_k = t_1\gamma_1(k)$ with $t_1 = 2.78$ eV as nearest-neighbor in-plane hopping integral. The Hamiltonian H_{AA} represents the hopping of electrons from first layer to second layer and vice-versa with inter layer hopping energy $\epsilon_{k,\perp} = t_\perp|\gamma_\perp(k)|$. Here $t_\perp = 0.04$ and $|\gamma_\perp(k)|$ are the perpendicular hopping integral and interlayer dispersion. The total Hamiltonian is given by $H = H_1 + H_2 + H_{AA}$

3. Calculation of Green's functions and AFM gap equation for AA-BLG

In order to calculate the physical parameters, we calculate the four coupled electron Green's functions involving electrons of A site carbon atom and they are defined as

$A_{\alpha,\beta}(k,\omega) = \ll a_{\alpha,k,\sigma}\; ; a^{\dagger}_{\beta,k,\sigma} \gg_{\omega}$, where $\alpha = 1{,}2$ for two layers and $\beta = 1-4$ for four Green's function. Similarly Green's functions involving electrons of B site carbon atoms are defined by $B_{\alpha,\beta}(k,\omega) = \ll b_{\alpha,k,\sigma}\; ; b^{\dagger}_{\beta,k,\sigma} \gg_{\omega}$. The coupled Green's functions are calculated by Zubarev's technique. For first layer at A site, we find $A_{1,1}(k,\omega) = \frac{a_{22}}{2\pi|D(\omega)|}$ and for first layer at B site, we find $B_{1,1}(k,\omega) = \frac{b_{22}}{2\pi|D(\omega)|}$. Equating the denominator term to zero i.e. $|D(\omega)| = 0$, we get the quasi-particle band dispersion energies $\omega_{\alpha,s}(k)$ which are given below

$$\omega_{\alpha,s}(k) = \mu - (-1)^s\sqrt{A_k - 2(-1)^{\alpha}B_k}\;,\; \alpha\;\&\; s = 1{,}2 \quad (4)$$

where $A_k = \frac{V^2}{4} + \Delta_A^2 + |\epsilon_k|^2 + |\epsilon_{k\perp}|^2$, $B_k = \sqrt{\frac{V^2}{4}\Delta_A^2 + |\epsilon_k|^2 \left(|\epsilon_{k\perp}|^2 + \frac{V^2}{4}\right)}$. The AFM gap equation is written as

$$\Delta_A = \frac{S}{(2\pi)^2} \iint dk_x dk_y \left[\left(< n_{1,\downarrow}^b > - < n_{1,\uparrow}^a > \right) - \left(< n_{2,\uparrow}^b > - < n_{2,\downarrow}^a > \right) \right] \quad (5)$$

where $< n_{\alpha,\sigma}^{\gamma} >$ represents the electron densities at different sites $\gamma = A, B$, and for both layers ($\alpha = 1,2$) for electron spin (σ). While doing all the calculations, the momenta are shifted to appropriate Dirac points lying on the Fermi level. All the parameters appearing in the calculation are scaled by nearest-neighbor hopping integral t_1. The reduced parameters are written as: the site energy at A site ea = $\frac{\epsilon_a}{t_1}$, site energy at B site eb = $\frac{\epsilon_b}{t_1}$, impurity concentration x , impurity potential u = $\frac{U_0}{t_1}$, nearest- neighbor hopping integral $\tilde{t_1} = -1$, and band energy c1 = $\frac{\omega}{t_1}$, AFM gap $z = \frac{\Delta_A}{t_1}$ and gate potential $v = \frac{V}{t_1}$.

4. Results and Discussion

The gate potential (v) applied between two layers of AA-stacked bilayer (AA-BLG) induces spin polarization at A and B sublattices on both the layers due to impurity effect . The AFM magnetic gap for the first layer given in equation (4) is computed self-consistently for different values of impurity potential as shown in figure 1. The electron doping by nitrogen impurity introduces an attractive impurity potential (i.e. $U_0 < 0$), while the hole doping by boron impurity introduces a repulsive potential (i.e. $U_0 > 0$) at the impurity site. In the present study we introduce hole doping by boron atoms with repulsive potential $U_0 = ut_1 = 0.855 * 2.78 = 2.377$ eV. For given gate potential $v = 0.04$ and impurity potential $u = 0.855$, the AFM gap ($z = 0.13$ at $t = 0$) gradually increases with temperatures, attains its peak value at a temperature $t = 0.85$ and then gradually decreases to zero at Neel temperatures $t_N \cong 1.22$ exhibiting mean-field behavior at higher temperatures. The AFM gap exhibiting similar temperature dependence with increase of Coulomb energy. However, the AFM gap is enhanced with increase of impurity energy throughout the temperature range exhibiting a sharp drop at t_N showing the robust character if the magnetic transition from the anti-ferromagnetic to paramagnetic phase. It is to note further that the AFM gap is suppressed with decrease of impurity energy and is finally suppressed at low temperature showing the paramagnetic phase and there by exhibiting the reentrant behavior (See figure1). It is noteworthy to mention that the anti-ferromagnetic Neel temperature in AA-BLG is much higher

compared to the Neel temperature calculated for monolayer graphene-on-substrate [15]

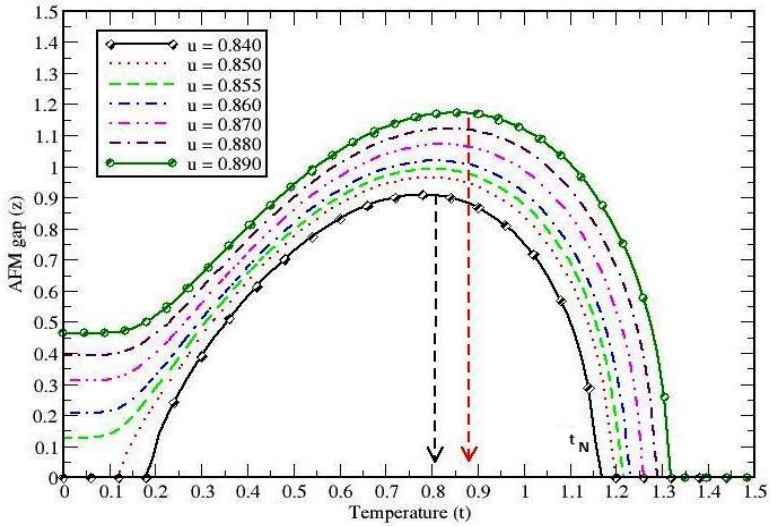

Fig. 1. shows the pot of AFM gap (z) vs. temperature (t) for different impurity potential $u = 0.855, 0.870, 0.880$ at fixed gate potential $v = 0.04$.

5. Conclusions

We have reported here the tight-binding model study of the on-site of anti-ferromagnetic order in AA-stacked BLG due to presence of gating potential and impurity interaction potential. The sub-lattice AFM magnetization of the system is calculated by Green's function technique and computed self-consistently. The effect of impurity interaction on AFM gap is reported in the present work. The temperature dependent AFM gap in AA-BLG is suppressed with decrease of impurity potential throughout the temperature range exhibiting robust magnetic order near Neel temperature. On further decreasing impurity potential, we find that the AFM gap exhibits re-entrant behavior at lower temperature having two Neel temperature. It is noteworthy we have recently, the tight-binding model study of magnetic spin susceptibility [16, 17], dielectric constant [18], electron specific heat [19]. The role of electron-phonon interaction on charge gap [20], ferromagnetism [21, 22], anti-ferromagnetism [23] and paramagnetism [24,25] for doped monolayer graphene on-substrate based on tight-binding calculation.

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