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Effects of Substrate and Coulomb Correlation on Ferromagnetism in Graphene

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Abstract. We report here a tight-binding model calculation taking into account of ferromagnetic order in graphene-on-substrate. The repulsive Coulomb interaction is considered within a mean-field model taking into account of the ferromagnetic moments at each sub-lattice of the honeycomb lattice. The sub-lattice magnetizations are calculated by Zubarev's Green function technique and are solved self-consistently.

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Keywords- Graphene, Ferromagnetism, Electron-electron interaction, Tight binding model

1. Introduction

The most phenomenal findings in solid state physics is graphene in the last decade [1, 2]. The graphene is a 2-D crystal material which consists of carbon atoms with sp2 hybridization. In free form it does not show the structural long-range order due to its low dimensionality, as per the Hohenberg-Mermin-Wagner (HMW) theorem [3]. The graphene exists in a flat shape surface at low temperature because of non-linear effect or in the existence of substrate induced gap or impurities that separate specifically the translational symmetry perpendicular to the graphene plane [4]. Graphene has very little ferromagnetic behavior at room temperature in pure form. The first principle calculations and tight-binding model studies have been applied for magnetism in such systems [5, 6]. The concept of Coulomb energy is very much important to recognize the imperfection induced magnetism [7]. When pristine graphene is placed on a substrate, the electron of substrate atom interacts with the π-electron of graphene so that A sub-lattice is raised by energy $(+\Delta)$ and B sub-lattice is suppressed by energy $(-\Delta)$. This produces difference in electron density at the two sub-lattices

leading to charge gap in the system [8]. The pristine graphene is a zero band gap semiconductor with zero electron density at the Fermi level. There exists finite electron density of state at Fermi level due substrate effect and the added impurities in graphene. Now graphene exhibits magnetism in the form of antiferromagnetic and ferromagnetic orders due to electron-electron interaction [9]. In continuation of this work, we have considered here the on-site electron-electron interaction within a mean-field approximation incorporating sub-lattice magnetizations at A and B sub-lattice sites. Earlier, we have reported the effect of nitrogen doping on sub-lattice ferromagnetism [10] and the effect band filling on FM sub-lattice magnetizations in graphene-on-substrate [11]. We report here the effect of substrate and Coulomb energy on temperature dependent sub-lattice magnetizations(m_a, m_b).

2. Tight-Binding Model Hamiltonian

The Hamiltonian consisting of nearest-neighbor (NN) hopping, next nearest neighbor (NNN) hopping and next to next nearest neighbor (NNNN) hopping of π-electrons is written as,

$$H_0 = \sum_{k,\sigma} [\, \varepsilon_{a,k}\ a^{\dagger}_{k,\sigma} a_{k,\sigma} + \varepsilon_{b,k} b^{\dagger}_{k,\sigma} b_{k,\sigma}] + \sum_{k,\sigma}[\, \varepsilon_{13}(k)\ a^{\dagger}_{k,\sigma} b_{k,\sigma} + \varepsilon^{*}_{13}(k)\ b^{\dagger}_{k,\sigma} a_{k,\sigma}\,] \quad (1)$$

where $\varepsilon_{a,k} = \varepsilon_a - \mu + \Delta + \varepsilon_{2k}$, $\varepsilon_{b,k} = \varepsilon_b - \mu - \Delta + \varepsilon_{2k}$ and $\varepsilon_{13}(k) = \varepsilon_{1k} + \varepsilon_{3k}$. The site energies ε_a and ε_b at A and B sub lattices are modified by chemical potential (μ), substrate induced gap (Δ), and NNN hopping energy (ε_{2k}). The band dispersions are $\varepsilon_{1k}, \varepsilon_{2k}\ and\ \varepsilon_{3k}$ for NN, NNN and NNNN hoppings. Here $a^{\dagger}_{k,\sigma}$ $(a_{k,\sigma})$ and $b^{\dagger}_{k,\sigma}$ $(b_{k,\sigma})$ are respectively the creation (annihilation) electron operators at A and B sub-lattices having momentum $\vec{k}$ and spin σ. The electron-electron interaction for A and B sub lattices is given by,

$$H_U = U \sum_i a^{\dagger}_{i\downarrow} a_{i\downarrow}\, a^{\dagger}_{i\uparrow} a_{i\uparrow} + U \sum_i b^{\dagger}_{i\downarrow} b_{i\downarrow}\, b^{\dagger}_{i\uparrow} b_{i\uparrow} \quad (2)$$

The ferromagnetism (FM) arises, when net magnetization in both the sub-lattices are in same direction and the average electron occupancy within the mean-field approach appears in general as, $\langle c^{\dagger}_{i,\sigma}\, c_{i,\sigma}\rangle = \left(\frac{n}{2} + \frac{\sigma m}{2}\right)$ where n and m are respectively the electron density and magnetization with σ taking +1(-1) for up(down) spins.

3. Calculation of Sub-lattice Magnetizations

The Green's functions for A site electron operator can be defined as,

$$A_1(k,\omega) = \ll a_{k,\sigma}; a_{k,\sigma}^{\dagger} \gg_{\omega} ; A_2(k,\omega) = \ll b_{k,\sigma}; a_{k,\sigma}^{\dagger} \gg_{\omega} \quad (3)$$

By using Zubarev Green's function technique, the final expressions of the above Green's functions are,

$$A_1(k,\omega) = \frac{1}{2\pi} \frac{\left(\omega - \epsilon_{b,\sigma}(k)\right)}{|D_\sigma(\omega)|}; \quad A_2(k,\omega) = \frac{1}{2\pi} \frac{\epsilon_{13}^{*}(k)}{|D_\sigma(\omega)|} \quad (4)$$

Similarly, the Green's functions for B site electron operators can be written as,

$$B_1(k,\omega) = \frac{1}{2\pi} \frac{\left(\omega - \epsilon_{a,\sigma}(k)\right)}{|D_\sigma(\omega)|}; \quad B_2(k,\omega) = \frac{1}{2\pi} \frac{\epsilon_{13}(k)}{|D_\sigma(\omega)|} \quad (5)$$

The FM magnetization(m_a) at A sub- lattice and FM magnetization (m_b) at B sub- lattice are written as,

$$m_a = \frac{1}{N}\sum_k \left(\langle a_{k,\uparrow}^{\dagger} a_{k,\uparrow}\rangle - \langle a_{k,\downarrow}^{\dagger} a_{k,\downarrow}\rangle\right)$$

and

$$m_b = \frac{1}{N}\sum_k \left(\langle b_{k,\uparrow}^{\dagger} b_{k,\uparrow}\rangle - \langle b_{k,\downarrow}^{\dagger} b_{k,\downarrow}\rangle\right) \quad (6)$$

The physical quantities are made dimensionless by NN hopping integral $t_1 \equiv 2.78eV$. The parameters are: the Coulomb energy $= \frac{U}{t_1}$, substrate induced gap $d_1 = \frac{\Delta}{t_1}$ and temperature $t = \frac{k_B T}{t_1}$.

4. Results and Discussion

The FM magnetizations (m_a, m_b) defined in equation (6) are calculated from the Green's functions and computed self-consistently for 110×110 grid points of electron momentum. The fig 1 shows the effect of substrate induced gap on the temperature dependent sub-lattice magnetizations. In absence of substrate (i.e. for low values of substrate induced gap $d_1 = 0.001$), the sub-lattice magnetizations are equal $(i.e. m_a = m_b)$ indicating that two sub-lattices are equivalent in pristine graphene. Hence the magnetization exhibits a perfect mean-field behavior for $d_1 = 0.001$ with a Curie temperature $t_c = 0.135$ ($T_c \approx 3753k$). With increase of substrate induced gap, the two sub lattices become more and more inequivalent giving rise to two different sub-lattice magnetizations $(m_a, m_b\ with\ m_a < m_b)$. With increase of substrate gap, FM magnetization (m_b) is enhanced, while FM magnetization $(m_a)$is suppressed giving rise to two different Curie temperatures in graphene. Both the magnetizations exhibit perfect mean-field behavior with ferromagnetic transition

in graphene-on-substrate. For substrate induced gap $d_1 = 0.09$, the two Curie temperatures are $t_c^a \approx 0.97$ *and* $t_c^b \approx 0.175$

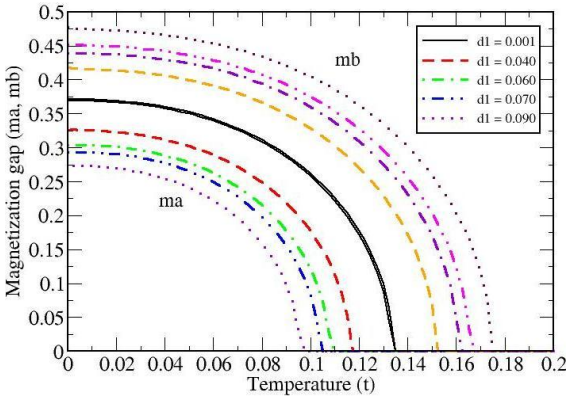

Fig. 1. The plot of FM magnetizations gap vs. temperature (t) for different values of substrate induced gap $(d_1 = 0.01 - 0.090)$ at fixed Coulomb potential $(u = 1.86)$ and electron density$(n = 1)$.

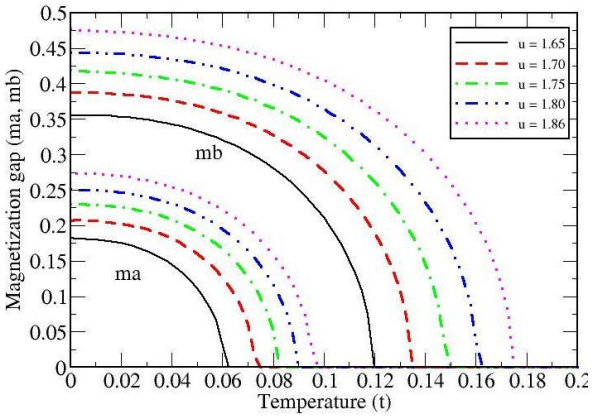

Fig. 2. The plot of FM magnetizations gap vs. temperature (t) for different values of Coulomb potential $(u = 1.65,1.70,1.75,1.80,1.86)$ at fixed substrate induced gap $(d_1 = 0.090)$ and electron density $(n = 1)$.

Figure 2 shows the effect of Coulomb energy on temperature dependent sub-lattice magnetizations. For a given Coulomb energy $u = 1.65$, the sub-lattice magnetizations exhibit perfect mean-field behavior with $m_a < m_b$. Both the sub-lattice magnetizations are enhanced throughout the temperature with increase of Coulomb energy from $u = 1.65 - 1.86$. Simultaneously the Curie temperatures

are enhanced with Coulomb energy exhibiting ferromagnetic transition in ferromagnetic state.

5. Conclusions

We report here a tight-binding study of FM magnetization in graphene due to the effects of substrate induced gap and Coulomb energy. The substrate induced gap induces two different types of magnetizations with $\mathbf{m_a} < \mathbf{m_b}$. Here the sub-lattice magnetization ($\boldsymbol{m_b}$)is enhanced with substrate induced gap, while ($\mathbf{m_a}$)is suppressed. The Coulomb correlation energy enhances both the sub-lattice magnetizations with enhancement of Curie temperatures. The electron density at carbon sites also enhances the sub-lattice magnetizations. We have reported earlier the effect of impurity on ferromagnetic order in graphene [10] and the interplay of Coulomb interaction and electron density in the ferromagnetic state in graphene [11]. Gouda et.al [12] have reported the doping and substrate effects on anti-ferromagnetic order in graphene-on-substrate.

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