

Density of States of Twisted Bilayer Graphene at Low Energy

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Abstract— We report the calculation of the Density of States (DOS) in Twisted Bilayer Graphene (TBG) system for low energy range near Fermi level using commensurate rotation of 1.16° , 1.79° and 3.48° . We obtain a logarithmic behaviour of DOS showing that van Hove Singularities (VHS) are occurred in this system and its position depends on twisted angle. This behaviour coming from the saddle points (SP) of band dispersion of TBG. The position of VHS will move away from Fermi level along with the increase of twisted angle. This result can be used to calculate others physical quantities such as optical conductivity or critical temperature of superconductivity that may occur in TBG.

Keywords – Density of States, Twisted Bilayer Graphene, Low Energy.

I. INTRODUCTION

Since first time isolated in 2004, Graphene has attracted a lot of interest from physicist to study its unique properties such as ballistic electron transport, quantum Hall effect and chiral tunneling[1,2]. Recently, study in multilayer Graphene is more attractive since the electronic properties of Graphene can be modified by piling up a few layers[3]. More interesting properties arise in Twisted Bilayer Graphene (TBG) system, in which two adjacent Graphene layers forms Bernal Stacking and rotated with respect to the others[3,4,5]. It has been known that van Hove Singularity (VHS) occurred in TBG[6] which drives the speculation that superconductivity maybe manifest in this system[7,8]. For small rotation or twisted angle, $\theta \leq 10^\circ$, we can modify the position of VHS by tuning the commensurate rotation. This methods of tuning never seen in other materials[4,5,6].

In this paper we report calculation of the Density of States (DOS) in TBG system. We assume that the TBG system has the same behaviour as the Pristine Graphene Monolayer (PGM), whereas the Fermi level located on Dirac Point. From this calculation we obtain logarithmic behaviour of DOS showing that VHS are occurred in this system and its position depends on twisted angle.

II. METHODS

In order to obtain DOS, we calculate the magnitude of group velocity of Dirac Fermion. The group velocity can be calculated via divergence from the dispersion of energy $E(\vec{k})$:

$$\vec{v} = \frac{1}{\hbar} \nabla_{\vec{k}} E(\vec{k}), \quad (1)$$

where \hbar denotes Planck constant and $E(\vec{k})$ is given by [9]:

$$E(k_x, k_y) = \alpha(A^2 + B^2)^{1/2}, \quad (2)$$

where

$$\alpha = \pm \frac{2\hbar^2 v_f^2}{15t},$$

$$A = k_x^2 - k_y^2 - \frac{1}{4}\Delta K_x^2 + \frac{1}{4}\Delta K_y^2,$$

$$B = 2k_x k_y - \frac{1}{2}\Delta K_x \Delta K_y,$$

where t is interlayer coupling and (k_x, k_y) is two dimensional wave vector relative to the midpoint of the two Dirac Points[9]. The vector ΔK ($\Delta K_x, \Delta K_y$) is relative shift of the Dirac Points in the Brillouin Zone (BZ) (see Fig. 1) with[4,5]

$$\Delta K = \frac{8\pi}{3a_0} \sin\left(\frac{\theta}{2}\right), \quad (3)$$

where a_0 is a lattice constant of the Graphene monolayer ($\approx 2,46 \text{ \AA}$), θ is the angle of commensurate rotation, $\Delta K_x = \Delta K \sin(\theta/2)$ and $\Delta K_y = \Delta K \cos(\theta/2)$ [4,5,7].

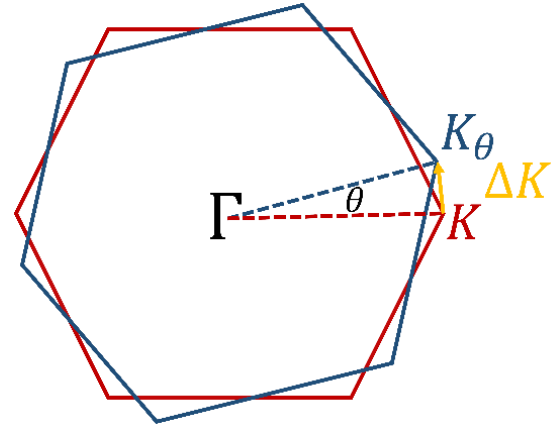


Figure 1. BZ of TBG

DOS can be calculated via (4) below :

$$D(E) = \frac{1}{4\pi^3 N \hbar} \int \frac{dl}{|\vec{v}|} \quad (4)$$

where dl is the element of length in the surface of energy and N is a number of unit cell over volume or surface area.

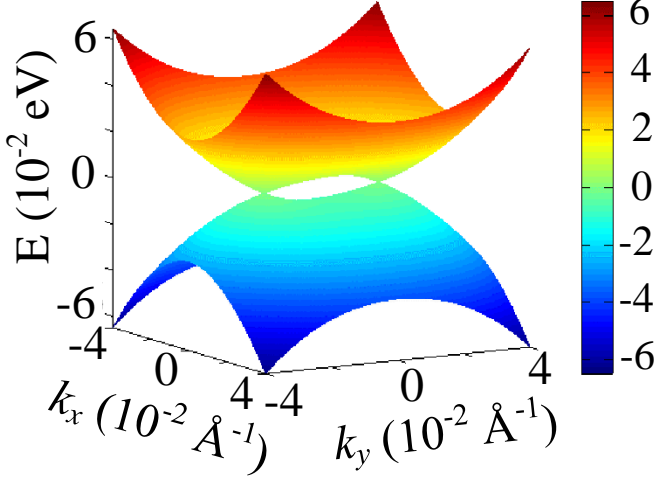


Figure 2. DE of TBG for the angle of commensurate rotation 1.16° .

III. RESULTS

The dispersion energy (DE) of TBG in (2) showing two split Dirac Cones with two VHS in the middle (see Fig. 2). Fig. 2 shows DE for the angle 1.16° . Fig. 3a and 3b show saddle points (SP) in the valence band and conduction band respectively, which is the cause of VHS occurrence. We change the scaling factor (α) in (2) from 2 becomes 99.24 to match VHS with the data of experiments (6 meV from Dirac Points) [6].

From (1) and (2), one can obtain the magnitude of group velocity which is given by :

$$|\vec{v}| = \frac{2\alpha\sqrt{k_x^2 + k_y^2}}{\hbar}. \quad (5)$$

Using (4) and (5), one can derive DOS as follow

$$D(E) = \frac{1}{16\alpha\pi^3 N} \left(\ln \left| \frac{\beta\alpha^2 + E_f^2}{\beta\alpha^2 + E^2} \right| \right),$$

$$\beta = -2 \left(A_1(k_x^2 - k_y^2) + B_1(2k_x k_y) \right) - \frac{1}{16} |\Delta K|^4, \quad (6)$$

where

$$A_1 = -\frac{1}{4} \Delta K_x^2 + \frac{1}{4} \Delta K_y^2, \quad B_1 = -\frac{1}{2} \Delta K_x \Delta K_y.$$

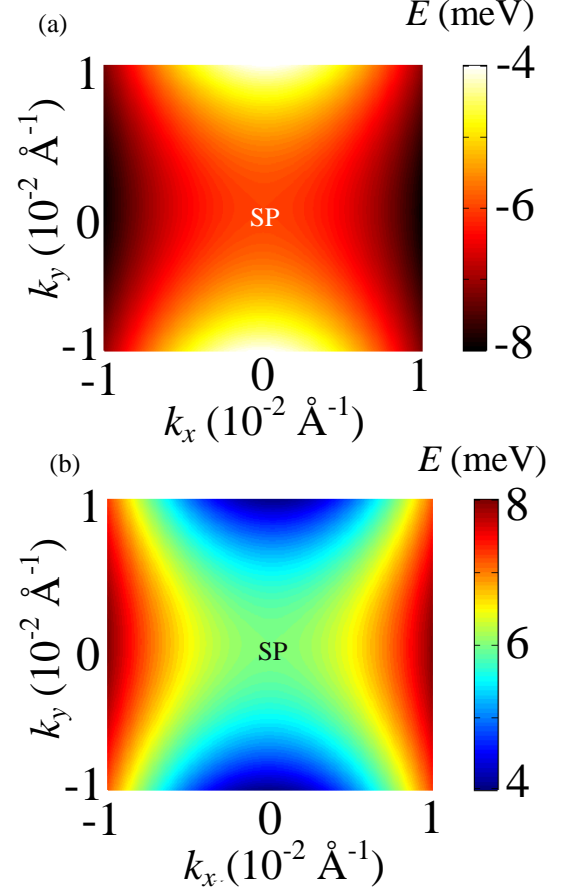


Figure 3. Saddle Points (SP) in the valence band (a) and conduction band (b) for the angle of rotation 1.16° .

In this calculation we assume that TBG model has the same behaviour as PGM in which the Fermi Level is located at the Dirac Points. Fig. 4 shows the plot of DOS derive from (6). In this figure, VHS is present indicated by the logarithmic shape of DOS at particular energy in the valence band and the conduction band. For the rotation angle of 1.79° , we change the scaling factor to 239.2 correspond to the VHS position about 41 meV from Dirac Points. Similar to rotation angle of 3.48° the scaling factor set to 436.6 where, as a consequence, VHS is placed on 215 meV from Dirac Points[6]. In general, commensurate rotation angle tune the position of VHS

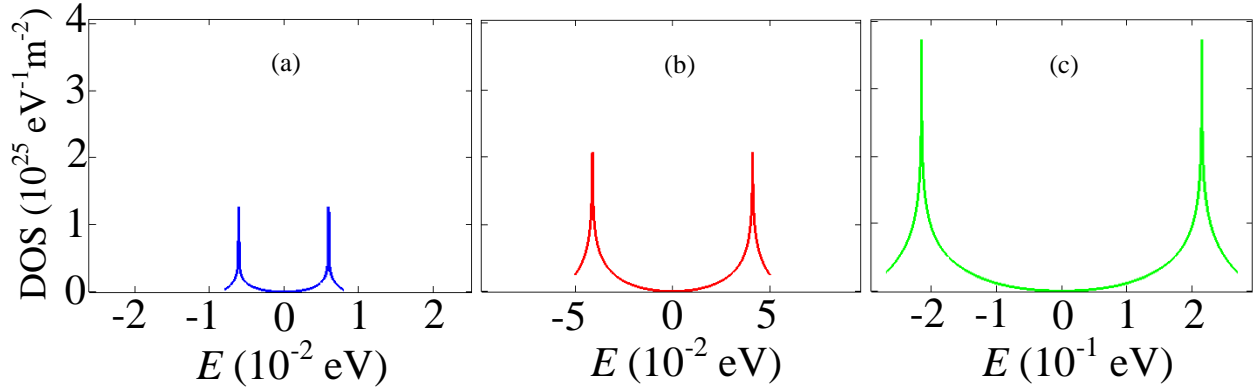


Figure 4. Plot of DOS for the angle of rotation (a) 1.16° (b) 1.79° and (c) 3.48° .

IV. CONCLUSION

In conclusion we have reported the calculation of DOS for TBG system. We have shown that DOS of TBG has logarithmic behaviour known as VHS in the valence band and conduction band, respectively. These two peaks are related to the occurrence of SP in DOS.

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