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The Possibility of Superconductivity in Twisted Bilayer Graphene

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Abstract. We discuss the possibility of superconductivity in Twisted Bilayer Graphene (TBG). In this study we use TBG model with commensurate rotation θ=1.16^{o} in which the van-Hove singularities (VHS) arise at 6 meV from the Fermi level. We use BCS standard formula that include Density of States (DOS) to calculate the critical temperature (T_C). Based on our calculation we predict that superconductivity will not arise in Pristine TBG because pairing potential has infinity value. In this situation, Dirac Fermions do not interact with each other since they do not form the bound states. Superconductvity may arise when the Fermi level is shifted towards the VHS. Based on this calculation, we predict that$T_C$has value between 0.04 K and 0.12 K. The low value of T_C is due to highly energetic of in plane phonon vibration which reduce the effective electron-phonon coupling. We conclude that doped TBG is candidate for Dirac Fermion superconductor.
Keywords : Superconductivity, Twisted Bilayer Graphene, Dirac Fermion.

INTRODUCTION

Since first time isolated in 2004, Graphene has attracted a lot of interest from physicist to study its unique physical properties such as ballistic electron transport, quantum Hall effect and chiral tunneling[1,2]. Unfortunately superconductivity is not one of special properties belongs to Pristine Graphene (PG)[3].The arguments that widely discussed regarding to non superconducting properties in PG are the vanishing of Density of States (DOS) at Fermi level and the absence of electron-electron screening[4]. A lot of suggestions have been proposed in order to make Graphene becomes superconductor such as the use of proximity effect in which Graphene is in contact with superconducting material[5]. Another suggestion is to doped Graphene with alkali metals like Lithium [4,6] or to highly doped by K and Ca[7]. In this manner van Hove Singularities (VHS) can be tuned to be in the vicinity of the Fermi level.The VHS is related to huge number of DOS of electron, thus enhancing probabilityof superconductivity in Graphene[7].

The presence of VHS is observed in Twisted Bilayer Graphene (TBG) system. In this system Graphene layers forms Bernal stacking and are rotated with respect to the others[8,9,10]. For small rotation of twisted angle ($\theta \leq 10^0$), we can modify the position of VHS by tuning the commensurate rotation[9,10,11]. It has been known that the smallest distance between VHS is 12 meV in TBG with angle of rotation 1.16^0[11]. Assuming Fermi level lies in Dirac Points, the distance from VHS to Fermi level will be 6 meV. We predict that superconductivity may arise in TBG system since the position of VHS is very close to Fermi level. In this situation, the interactions (i.e. between Dirac Fermions) will be magnified due to the enhancement of DOS, resulting instabilities and will give rise to new state of matter including superconductivity.In this work, we use BCS standard formula to calculate the critical temperature (T_C) with the input of DOS from TBG system.

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CALCULATION METHODS

Weak-coupling approximation (BCS theory) is used to predict superconductivity that may arise in TBG. In order to find critical temperature we useBCS gap equation which is given by [12]:

$$\frac{1}{V} = \int_{0}^{\hbar\omega_D} D(E)\tanh\left(\frac{E}{2k_B T_C}\right)\frac{dE}{E}, \tag{1}$$

where ω_D is Debye frequency, V is pairing potential, k_B is Boltzman constant and $D(E)$ is DOS of TBG. The DOS of TBG has been calculated previously and is given by[13] :

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

where $\alpha = \pm 99.24\hbar^2 v_F^2/15t$, $\beta = -2\left(A_1\left(k_x^2 - k_y^2\right) + B_1\left(2k_x k_y\right)\right) - 1/16\left|\Delta K\right|^4$, $A_1 = -1/4\left(\Delta K_x^2 - \Delta K_y^2\right)$ $B_1 = -1/2\left(\Delta K_x \Delta K_y\right)$, t is interlayer coupling and $\left(k_x, k_y\right)$ is two dimensional wave vector relative to the mid point of the two Dirac points. The vector ΔK $\left(\Delta K_x, \Delta K_y\right)$ describes the relative shift of the Dirac Points in the Brillouin Zone with $\Delta K = \left(8\pi/3a_0\right)\left(\sin\left(\theta/2\right)\right)$[12], where a_0 is a lattice constant of Graphene (≈ 2.46 Å), θ is the angle of commensurate rotation, $\Delta K_x = \Delta K \sin\left(\theta/2\right)$ and $\Delta K_y = \Delta K \cos\left(\theta/2\right)$. Figure 1 shows the plot of DOS for the angle of rotation of 1.16^0.

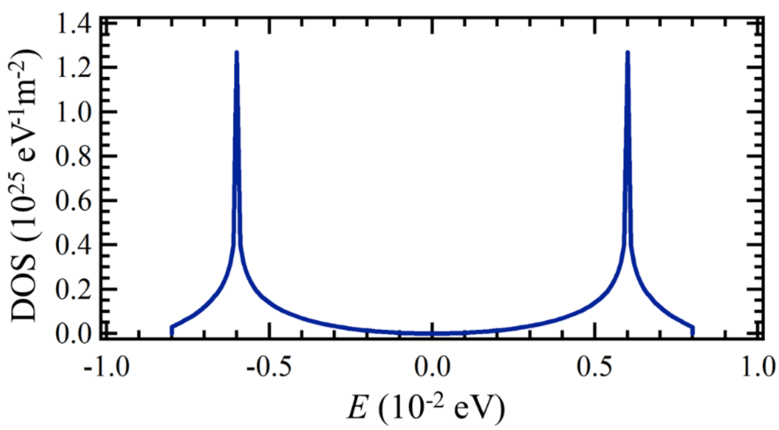

Figure 1. Plot of DOS for the angle of rotation of 1.16^0.

RESULT AND DISCUSSION

The critical temperature or T_C from TBG superconductivity can be calculated by inserting equation (2) into equation (1), yielding:

$$\frac{1}{N_0 V} = \ln\left(\frac{4e^{\delta}\hbar\omega_D}{2\pi k_B T}\right)\left(\ln\left(\frac{B_2}{B_2 + \left(\hbar\omega_D/k_B T\right)^2}\right) + \ln\left(\frac{B_2 + \left(\hbar\omega_D/k_B T\right)^2}{B_2}\right)\right) \tag{3}$$

From equation (3), It is obvious that we will have infinity pairing potential V as the right hand side of equation (3) becomes zero. This result can be interpreted as the Dirac Fermion could not be interact to each other, hence no bound states (i.e., Cooper Pairs) appear in Pristine TBG. Therefore we predict that superconductivity will never arise in Pristine TBG which is the same case as in Pristine Graphene. It can be mentioned that VHS location (i.e. 6 meV) is still not close enough to Fermi level.

In order to make TBG becomes superconductor one should makes VHS location exactly at the Fermi level. The Fermi level can be tuned to be at the VHS by using gate voltage [11]. This method is more easier as compared to doping TBG with another materials.In this method, Fermi level can be tuned close to VHS in the conduction band using electrons (related to negative gate voltage).Since VHS also occurred in the valence band then the Fermi level can be tuned also by hole (related to positive gate voltage) in order to move it to valence band. Figure 2a shows the DOS of TBG with positive gate voltage causing the Fermi level shifted to VHS in valence band (previously at -6 meV).

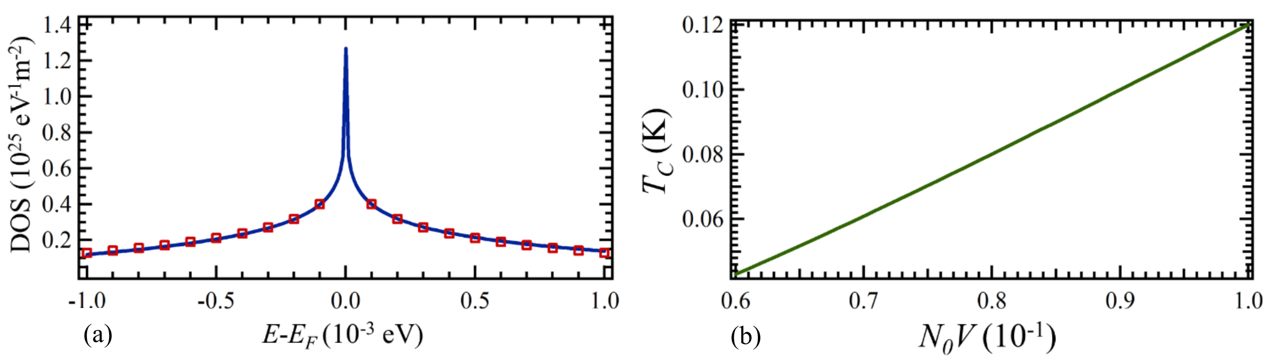

Figure 2. (a) Plot of DOS with the Fermi level located exactly at VHS in the valence band (b) Critical Temperature (T_c) as a function of coupling constant (N_0V).

The DOS shown in Fig.2a can be approximated by equation (4) (denoted as red square in Fig.2a) :

$$D(E) = N_0\left(\ln\left|\frac{E_1}{E}\right| + C\right), \tag{4}$$

where $N_0 = 1/16\alpha\pi^3 N, E_1 = 0.01$ and $C = -1.2$. The solution of BCS equation using DOS expressed in equation (4)is given by (see Ref.[12]):

$$k_B T_C = 1.36 E_1 \exp\left(C - \sqrt{\frac{2}{N_0 V} + \left(\ln\left(\frac{E_1}{\hbar\omega_D} + C\right)\right)^2 - 1}\right), \tag{5}$$

In equation (5) we use coupling constant $(N_0 V)$ value from 0.06 until 0.10 and Debye temperature (T_D) value of 2100 K (from Graphite[14]). T_D is related to phonon frequency through $\hbar\omega_D = k_B T_D$. The solution of equation (5) can be plotted as in Fig.2b which shows the coupling constant dependence of the critical temperature. The result shows that TBG with gate voltage behaves like good metalic based superconductor material. The example of good metallic based superconductor material with low T_C are Ti (0.39 K), Zn (0.88 K) and W (0.01 K). The low T_C in TBG system can be explained as followed: in normal state of the good metal the electrons were experiencing slight scattering by phonon, hence the interaction between electrons through phonon is less. Consequently, when the system is in superconducting state, the number of Cooper Pairs is less yielding to lower T_C. Moreover, it has been known that Graphene has high energetic phonon vibrations[3], which weaken the coupling of electrons with the phonon.

CONCLUSION

In conclusion, we have shown that Pristine TBG could not be a superconductor. The infinity value of pairing potential making the bound state of Cooper Pairs is very unlikely in Pristine TBG. TBG could be a superconductor when the system is doped by electron or hole using gate voltage so that the Fermi level placed on VHS. Our calculation shows that TBG with gate voltage has a critical temperature (T_C) between 0.04 K and 0.12 K which corresponds to coupling constant from 0.06 to 0.10.

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REFERENCES

1. A.H. Castro Neto, F. Guinea, N.M.R. Peres, K.S. Novoselov and A.K. Geim, Rev.Mod.Phys. **81**, 109 (2009).
2. K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V.Dubonos, I.V. Grigorieva and A.A. Firsov, Science, **306**, 666 (2004).
3. O.Vafek, Nature Phys. **8**, 111 (2012).
4. B.Uchoa and A.H. Castro Neto, Phys.Rev.Lett. **98**, 146801 (2007).
5. H.B. Heersche, P. Jarillo-Herrero, J.B. Oostinga,L.M.K. Vandersypen and A.F. Morpurgo, Nature **446**, 56 (2007).
6. G.Profeta, M. Calandra and F. Mauri, Nature Phys. **8**, 131 (2012).
7. J.L. McChesney, A. Bostwick, T. Ohta, T. Seyller, K. Horn, J. Gonzalez and E. Rotenberg, Phys.Rev.Lett. **104**, 136803 (2010).
8. E.S. Morel, P. Vargas, L. Chico and L. Brey, Phys.Rev.B **84**, 195421 (2011).
9. J.M.B. Lopes dos Santos, N.M.R. Peres and A.H. Castro Neto, Phys.Rev.Lett. **99**, 256802 (2007).
10. J.M.B. Lopes dos Santos, N.M.R. Peres and A.H. Castro Neto, Phys.Rev.B **86**, 155449 (2012).
11. G. Li, A. Luican, J.M.B. Lopes dos Santos, A.H. Castro Neto, A. Reina, J. Kong and E.Y. Andrei, Nature Phys. **6**, 109 (2010).
12. A.G. Goicochea, Phys.Rev.B **49**, 6864 (1994).
13. M.N. Manaf, I. Santoso and A. Hermanto, Proceedings of 2014 International Conference of Physics, Yogyakarta, 2014, edited by I. Santoso, A. Kusumaatmaja and F. Nugroho (Atlantis Press, Paris, 2014), p. 19 (doi:10.2991/icp-14.2014.5).
14. E. Pop, V. Varshney and A.K. Roy, MRS Bull. **37**, 1273.