Electron states in graphene nano-disks

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Abstract— **Extensive studies have been done on graphene nano-ribbons (GNRs). However, there are few studies on electronic properties of graphene nano-disks (GNDs). This paper focuses on electron states of GNDs and investigated different types. Most previously reported researches which have been done regarding these systems are usually limited to single particle picture through the tight bonding approach and some of them are based on the Density Functional Theory (DFT) and include some partial effects of these many-body systems. Here, our investigation includes full two-particle viewpoint with consideration of spin and electron-electron (e-e) interaction.**

Keywords-graphene nano-disks; spin; electron-electron interaction; Identical particles principle.

I. INTRODUCTION

Graphene is a 2D carbon crystal which has attracted much attention due to its unique properties collection. High carrier mobility, high elasticity and thermal conductivity and being 2 dimensional are some of its properties [1]. Having one atom thickness makes graphene a suitable candidate for the new generation of devices. This material can be used in electronics [2][3] optoelectronics [4][5] and spintronics [6][7][8].
Due to different properties of GNDs compared to the GNRs, these materials can be used for light absorption and creating exciton in photovoltaics [9]. Some properties like high carrier mobility and long spin coherence can lead to making effective spintronic devices based on graphene nano-structures such as nano-disks [10]. Several applications have been explored for these graphene disks [11][12].

In this paper, we have focused on electron states of the GNDs and have investigated the smallest disk (C_3), then C_6, C_{24} and the disk with 54 carbon atoms (C_{54}). Previous works in this field have been limited to the single particle viewpoint and were based on tight binding model [13] or many-body effects have been seen by DFT which is based on single particle system with the averaging effects of many-body [14][15].
Our investigation contains the single particle viewpoint without spin, the single particle system with spin, two-particle picture without spin and e-e interaction, two-particle viewpoint with spin and without e-e interaction and finally two-particle viewpoint with spin and e-e interaction. In addition, simple and anti-symmetric states have been investigated.

In next section, we present different calculated states and show the differences caused by various approximations (such as neglecting spin and e-e interaction) in calculations. Finally, conclusions are presented in last section.

II. ELECTRON STATES CALCULATION

A. Single particle system

We can write the Hamiltonian of this system as

$$H = \sum_i \varepsilon_i c_i^\dagger c_i + \sum_{\langle i,j \rangle} t_{ij} c_i^\dagger c_j + h.c. \qquad (1)$$

where ε_i is the site energy, t_{ij} is the transfer energy, and $c_i^\dagger$ is the creation operator of the π electron at the site i.

In all calculations, we consider single-orbital and nearest neighborhood model for every carbon atom.
First of all, we calculate C_3 states and summarize the results in Table 1.

Table I. Electron states of nano-disk C_3

	State 1	State 2	State 3
First site	0.5774	0.7071	0.4082
Second site	0.5774	-0.7071	0.04082
Third site	0.5774	0	-0.8165
Energy (eV)	-5	3.4	3.4

As it can be seen in Table 1, two excited states are degenerated.

The colors represent different phases and their changing in two neighbor sites demonstrates the electron velocity during its movement between those neighbor sites.

Electron states of the C_3 are plotted in Fig. 1. Here, linear combinations of the two excited states have been plotted. Energy of the different levels for various GNDs in this approximation are shown in Table 2.

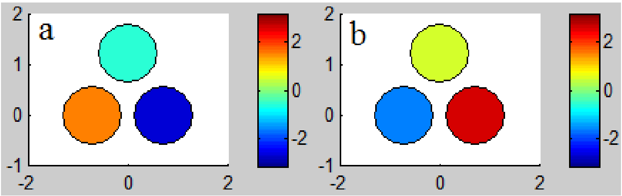

Figure 1. Electron states of C_3 a) $\frac{|\psi_2\rangle - i|\psi_3\rangle}{\sqrt{2}}$ b) $\frac{|\psi_2\rangle + i|\psi_3\rangle}{\sqrt{2}}$

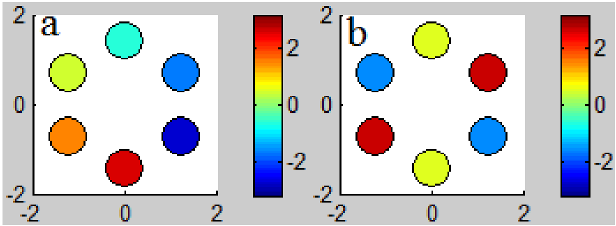

Figure 2. Electron states of C_6 a) $\frac{|\psi_2\rangle + i|\psi_3\rangle}{\sqrt{2}}$ b) $\frac{|\psi_4\rangle - i|\psi_5\rangle}{\sqrt{2}}$

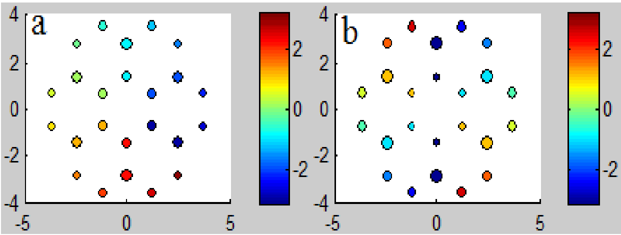

Figure 3. Electron states of C_{24} a) $\frac{|\psi_2\rangle + i|\psi_3\rangle}{\sqrt{2}}$ b) $\frac{|\psi_4\rangle - i|\psi_5\rangle}{\sqrt{2}}$

Table 2. - Energy of the electron states in various GNDs (C_3 , C_6 , C_{24} , C_{54}) - unit : eV

# of state	C_3	C_6	C_{24}	C_{54}
1	-5	-5	-6.89	-7.3643
2	3.4	-2.2	-5.6	-6.7391
3	3.4	-2.2	-5.6	-6.6903
4		3.4	-4.09	8.5432
5		3.4	-4.09	-5.9245
6		6.2	-3.709	-5.8665
7			-2.8	-5.6380
8			-2.2	-5
9			-2.2	-4.8716
10			-2.2	-4.5266
11			-0.909	-4.4548
12			-0.909	-3.8961
13			2.109	-3.8918
14			2.109	-3.3630
15			3.4	-3.2963
16			3.4	-3.2045
17			3.4	-2.8650
18			4	-2.8524
19			4.909	-2.3414
20			5.29	-1.3090
21			5.29	-1.2875
22			6.8	-0.9199
23			6.8	-0.3577
24			8.09	-0.1636
25				7.8903
26				7.8501
27				7.0665
28				7.0229
29				6.7556
30				1.5577
31				1.7283
32				2.3807
33				2.5090
34				2.6540
35				6.2
36				5.9995
37				5.6548
38				5.5403
39				5.0961
40				5.1032
41				3.4973
42				4.4963
43				4.44
44				4.2509
45				4.065
46				4.1224
47				3.4
48				-2.2
49				3.4
50				-2.2
51				-2.2
52				-2.2
53				3.4
54				3.4

The electron states have been plotted for other GNDs i.e. C_6, C_{24} and C_{54} in Fig. 2, 3, 4, respectively (only two states for every GND have been plotted).

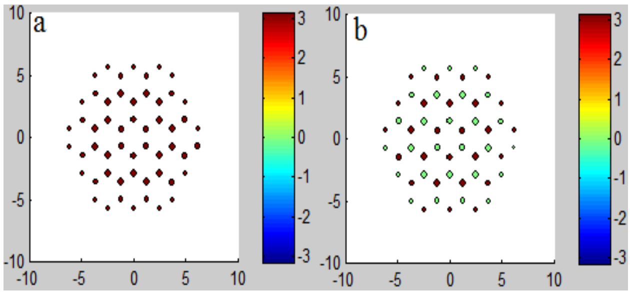

Figure 4. Electron states of C_{54} a) ground state *b)* an excited state.

The larger circle in a site means there is more probability of electron for electron to be in that site. Unlike other works, phase has been considered and plotted in addition to amplitude in our calculations and represents electron's velocity and its movement direction in every GND. For example, in Fig. 2, it can be seen that the electron state related to $\frac{|\psi_2\rangle + i|\psi_3\rangle}{\sqrt{2}}$ is slower in comparison with $\frac{|\psi_4\rangle - i|\psi_5\rangle}{\sqrt{2}}$; because in the Fig. 2(a), electron phase changes from minimum to maximum value once during a single rotation while for Fig. 2(b) it changes twice.

Moreover, we can conclude that the electron has certain direction of movement in every state which has been created by linear combination of two simple states. If new state has been made by summing of the two states, the direction is counter clockwise and if that has been created by subtracting of the those states, the movement direction of the electron is clockwise.

B. *Single particle states with consideration of spin*

The space of the electron's spin is two dimensional (2D) so spin state is shown by a 2D vector. Bases of this space are $|\uparrow\rangle = \begin{bmatrix}1\\0\end{bmatrix}, |\downarrow\rangle = \begin{bmatrix}0\\1\end{bmatrix}$ on S_z representation. The space of single-particle states with consideration of spin is obtained from multiplying spatial representation vector of the state by spin representation vector. Hamiltonian will be:

$$H = \sum_{i\sigma} \varepsilon_i c_{i\sigma}^{\dagger} c_{i\sigma} + \sum_{\langle i,j\rangle\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + h.c. \qquad (2)$$

In fig. 5 states $|1\uparrow\rangle, |1\downarrow\rangle$ are shown for the disk C_3. As expected they're identical in spatial representation and if there is not any term which is spin-dependent in Hamiltonian i.e. spin-orbit interaction, thus these two states have the same energy.

C. *Two independent particles states without consideration of spin*

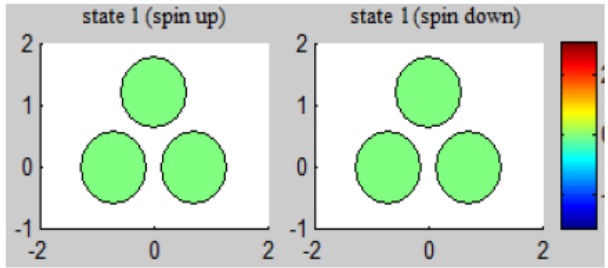

Figure 5. States $|1\uparrow\rangle, |1\downarrow\rangle$ of the disk C_3.

In this picture, the states are obtained from multiplying two single-particle states ($|1,2\rangle = |1\rangle \otimes |2\rangle$) and Hilbert space dimension is raised to the second power; e.g. for the disk C_{24}, will be equal to 576. Fig. 6 demonstrate these states' energy for two disks.

D. *Two independent particles states with consideration of spin*

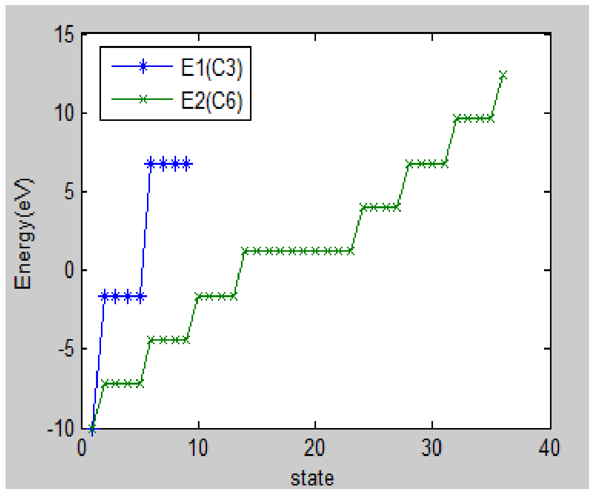

Figure 6. Energies of two independent particles states for the disks C_3 and C_6.

By considering the spin, Hilbert space will be four times larger and the states are obtained from multiplying corresponding single-particle states.

Again, one may say if there is not any spin-dependent term in Hamiltonian i.e. spin-spin interaction and spin-orbit interaction (almost invariably the magnitude of these terms is too small in comparison to the coulomb terms), these states energy will not be spin-dependent.

E. Two-particle states with electron-electron interaction and with consideration of spin

By considering e-e interaction, space dimension is not changed. However, interaction term will be added to the Hamiltonian.

$$H = \sum_{i\sigma} \varepsilon_i c_{i\sigma}^{\dagger} c_{i\sigma} + \sum_{\langle i,j \rangle \sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + h.c. + \sum_{\langle i,j \rangle \sigma} U_{ij} n_{i\sigma} n_{j\sigma} \tag{3}$$

Where U_{ij} is the coulomb interaction between site i and site j Fig.7 demonstrates the results for disk C_6 in this condition (with e-e interaction and spin) and previous results which are obtained without e-e interaction. As expected, the energies are shifted toward positive values and the shift is related to e-e interaction which is positive value.

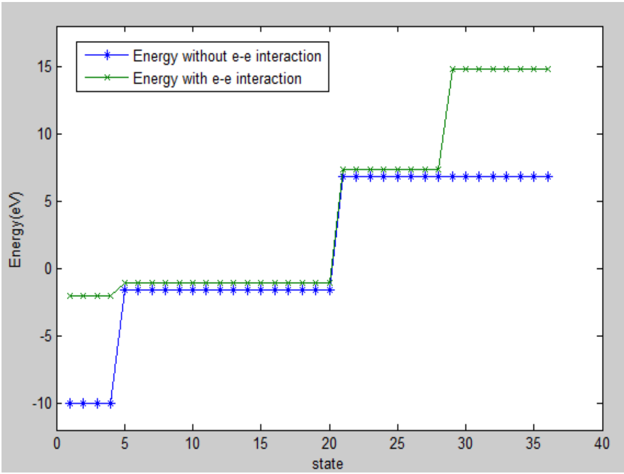

Figure 7. Energies of the disk C_6 states with and without consideration of e-e interaction.

F. Identical particles and Pauli exclusion principle

Generally, above-mentioned calculations neglect electrons' identicalness. If this truth is considered by performing anti-symmetric operation on the wave function, a significant change will occur in number of states in addition of their forms and energies. For instance, one can consider disk C_3. In this case, there are 15 different states instead of the 36.

In other words, six states vanish by considering the exclusion principle. The states are

$$|1\uparrow,1\uparrow\rangle, |2\uparrow,2\uparrow\rangle, |3\uparrow,3\uparrow\rangle, |1\downarrow,1\downarrow\rangle, |2\downarrow,2\downarrow\rangle, |3\downarrow,3\downarrow\rangle$$

Moreover, other 30 states will be paired two by two. Fig. 8 indicates energy of disk C_3 states from all the above viewpoints in a comparative way.

III. Conclusion

In this paper, electron in different GNDs states were investigated in various pictures. Single and two particle pictures with and without considering spin and e-e interaction were taken into consideration. For the different graphene disks, energies were calculated and electron states were plotted. Unlike other works, in this paper, phase of the states was considered in addition to their amplitude and effect of the phase is interpreted. Furthermore, electrons' identicalness and Pauli exclusion principle were considered and finally e-e interaction and exclusion principle effects on a GND energies were demonstrated. The difference in results was observed when one uses various approximations and this difference can be significant in some conditions.

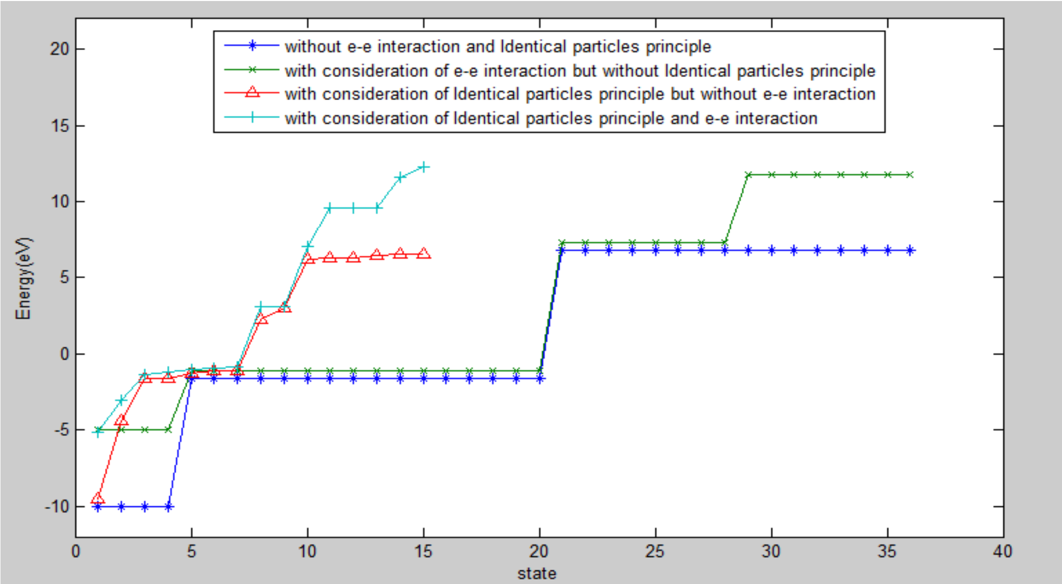

Figure 8. Energy of two electron states for disk C_3 with and without consideration of e-e interaction and with and without considering identical particles principle.

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