

## Computation of Energy Distribution as a Function of Wave-Vector ( $k$ ) for Specific CNT Configuration

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### ABSTRACT

In this paper, the energy dispersion relation has been calculated for certain configuration of single wall carbon nanotubes (SWNT) with respect to the wave vector ( $k$ ). The three types of SWNT are armchair, zigzag, and chiral, so the energy dispersion relation for them are calculated for different chiral vectors. Taking two chiral vectors for each type of CNT, so (7, 7), (10, 0) for armchair, for zigzag (7, 0), (10, 0), and (10, 5), (20, 5) for chiral.

### حساب توزيع الطاقة كدالة لمتجه الموجة ( $k$ ) لأنواع محددة من تركيب الانبوب الكربون النانوي

#### الخلاصة

في هذا البحث، تم حساب علاقة الطاقة المشتتة لتكوين معين للجدار الاحادي للانبوب النانوي للكربون. ان النوعان الرئيسيان للجدار الاحادي للانبوب النانوي للكربون هما الكرسي المسند، والمتعرج. ان علاقة الطاقة المشتتة للكرسي المسند والمتعرج حسب المتجه chiral (7,7), (7,0), (10,0), (10,5), (20,5)، على التوالي.

### INTRODUCTION

In 1991 Sumio Iijima of NEC discovered carbon nanotubes [1,2]. They are one of the most commonly mentioned building blocks of nanotechnology. The high aspect ratio is the main part that makes some of its property improved. The carbon nanotubes have long cylindrical structure with diameter at nm level and length at  $\mu\text{m}$  level which make their aspect ratio as high as 1000 or larger. There are many types of carbon nanotubes like single wall, double wall, and multi-wall. Single wall carbon nanotube (SWNT) are proposed to consist of a seamless cylinder of graphene sheet capped by hemispherical ends composed of hexagons [3]. It is represented by the pair of indices ( $n, m$ ) called the chiral vector as shown in Figure (1),  $C_h = na_1 + ma_2$ . The integers  $n$  and  $m$  denote

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the number of unit vectors along two directions in the honeycomb crystal lattice of a grapheme. If  $m=0$ , the nanotubes are called "zigzag". If  $n=m$ , the nanotubes are called "armchair". Otherwise, they are called "chiral". From those two basic parameters of carbon nanotube, many others nanotube geometrical parameters can be derived. Since the chiral vector gives the circumference of nanotube, the diameter of nanotube can be obtained as [8].

$$d_{NT} = \frac{|\vec{C}_h|}{\pi} = \frac{\sqrt{\vec{C}_h \cdot \vec{C}_h}}{\pi} = \frac{a\sqrt{n^2 + nm + m^2}}{\pi} \quad \dots (1)$$

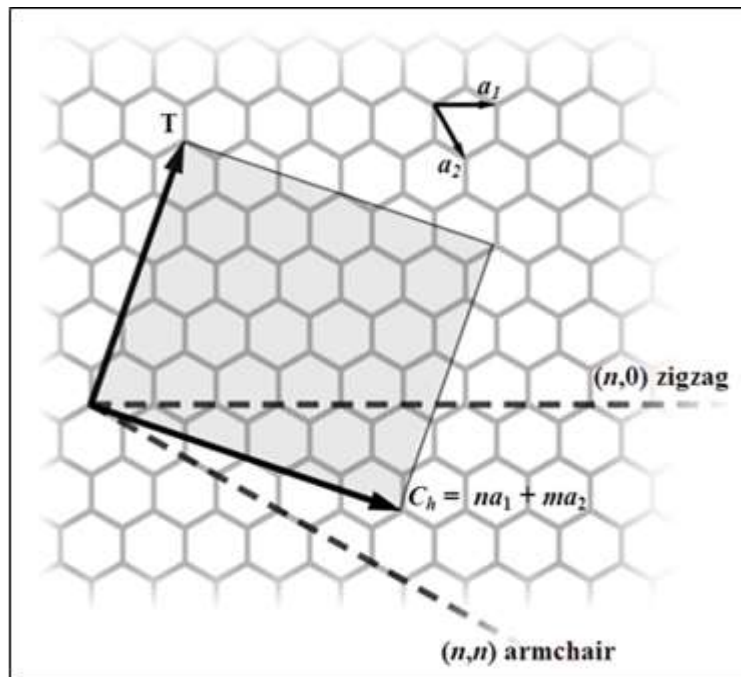


Figure (1) schematic of a two-dimensional grapheme sheet[5] .

## THEORY

The essence of the various calculations of the 1D electronic band structure is based on a tight binding or Hiickel calculation that neglects curvature of the nanotubes [6]. Since atomic orbitals are mostly localized, the wave functions in the lattice can be represented by a linear combination of the mostly localized orbital of the atom taking into account two carbon atom basis of the lattice, the wave function may be model as :

$$\Psi_j(\vec{k}, \vec{r}) = \sum_{j,j'=A,B} C_{jj'} \phi_{j'}(\vec{k}, \vec{r}) \quad \dots (2)$$

$$\phi_{AB}(\vec{k}, \vec{r}) = \frac{1}{\sqrt{N_{AB}}} \sum_{\vec{R}_{A,B}} e^{i\vec{k} \cdot \vec{r}} \phi(\vec{r} - \vec{R}_{A,B})$$

$$\dots (3)$$

Where  $n$  denote the number of Bloch function  $C_{jj'}$  are coefficients that must be found which weigh the Bloch function to the eigenfunction. The corresponding energy eigenvalue of eigenfunction states  $\phi_{A,B}$  are wave functions that satisfy Bloch equation.  $\phi$  are the waveforms of the atomic carbon  $p_z$  orbital and carbon coordinates  $\vec{R}_A$  and  $\vec{R}_B$  are basis atom positions translated through the lattice. The based on Schrödinger equation solution for energies and coefficients that determine the wave function is:

$$\hat{H}\vec{C}_i = E_i(\vec{k})\hat{S}\vec{C}_i \quad \dots (4)$$

where  $\hat{H}$  and  $\hat{S}$  are called transfer integral matrices and overlap integral matrices respectively, which are defined by[9].

$$H_{jj'} = \langle \psi_j | H | \psi_{j'} \rangle; S_{jj'} = \langle \psi_j | \psi_{j'} \rangle (j, j' = A, B) \quad \dots (5)$$

Because we have identical atoms in the basis set, we can take

$$H_{AA} = H_{BB} = 0 \quad \dots (6)$$

and

$$H_{AB} = H_{BA}^* = t.f(\vec{k}) = t(e^{ik_x a / \sqrt{3}} + e^{ik_x a / \sqrt{3}} \cos(k_y a / \sqrt{2})) \quad \dots (7)$$

where  $k_x, k_y$  is the wave vector along the direction of carbon nanotube axes. The transfer integral between the two neighboring atomic orbital is given by value  $t$ :

$$t = \langle \psi_A | H | \psi_B \rangle \quad \dots (8)$$

By taking the determine of equation Schrödinger and solving  $\hat{H}$  and  $\hat{S}$  as given above, the eigenvalues  $E_k$  are obtained as a function of ( $\vec{k}$ ) and  $w(\vec{k})$ .

$$E(\vec{k}) = \frac{\epsilon_{2p}}{1 \pm tw(\vec{k})} \quad \dots (9)$$

where

$$w(\vec{k}) = \sqrt{|f(\vec{k})|^2} = \sqrt{1 + 4 \cos\left(\frac{\sqrt{3}k_x a}{2}\right) \cos\left(\frac{k_y a}{2}\right) + 4 \cos^2\left(\frac{k_y a}{2}\right)} \quad \dots (10)$$

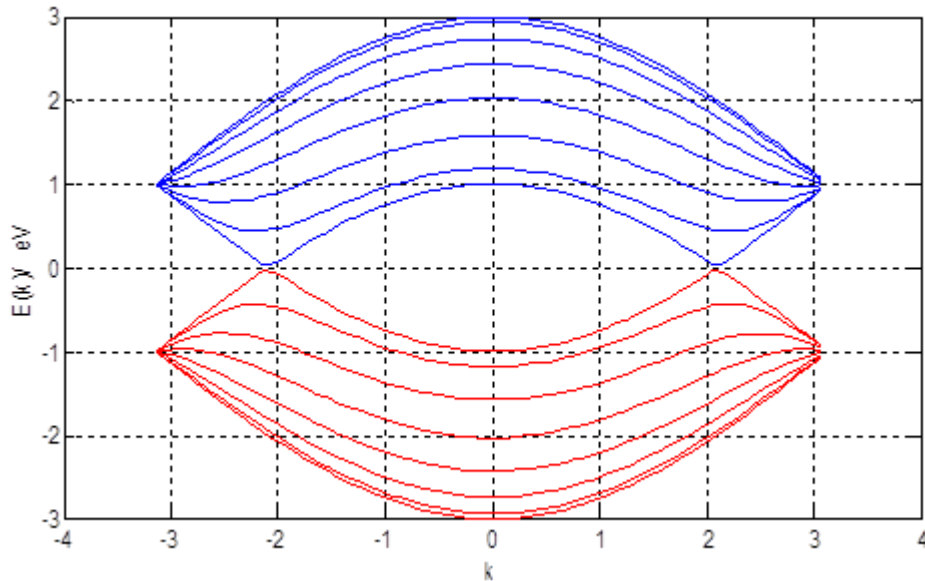
when  $\varepsilon_{2p} = 0$ , the dispersion relation becomes .

$$E_g(k_x, k_y) = \pm t \sqrt{1 + 4 \cos\left(\frac{\sqrt{3}k_x a}{2}\right) \cos\left(\frac{k_y a}{2}\right) + 4 \cos^2\left(\frac{k_y a}{2}\right)} \quad \dots (11)$$

where  $a$  is the lattice constant.

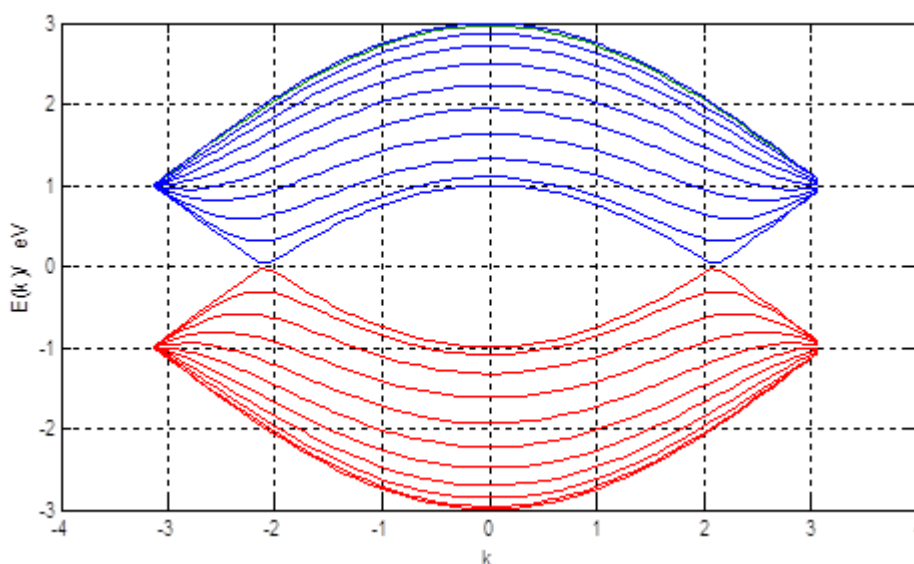
## RESULTS AND DISCUSSION

The energy dispersion relation of CNT was calculated by using MATLAB for the three types of nanotubes (armchair, zigzag, achiral). For the armchair carbon nanotubes The resulting calculated 1D energy dispersion relations  $E(k)$  for the (7, 7) armchair nanotube ( $N_x = 7$ ) are shown in Figure (2), where we see 8 dispersion relations for the conduction bands and an equal number for the valence bands. In each case, two bands are nondegenerate and six are doubly degenerate , leading to 14 levels in each case, consistent with the 14 hexagons around the circumference of the (7, 7) carbon nanotube.



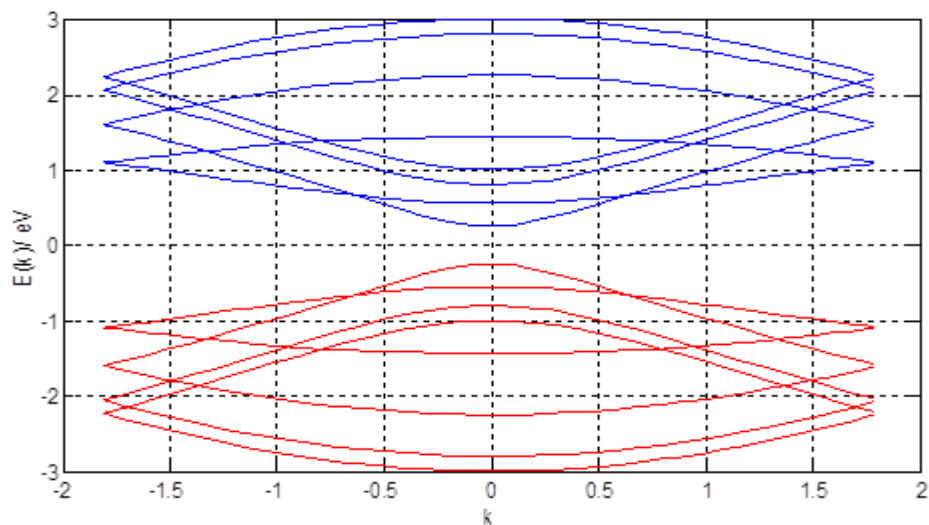
**Figure (2) One-dimensional energy dispersion relations for armchair (7,7) carbon nanotube.**

For all armchair tubules, the energy bands show a large degeneracy at the zone boundary, where  $ka_0=\pi$ . The valence and conduction bands in Figure (2) cross at a k point that is two thirds of the distance from  $k=0$  to the zone boundary at  $k = \pi/a_0$ . The crossing takes place at the Fermi level and the energy bands are symmetric for  $\pm k$  values. Because of the degeneracy point between the valence and conduction bands at the band crossing, the (7, 7) carbon nanotube will exhibit metallic conduction at finite temperatures, because only infinitesimal excitations are needed to excite carriers into the conduction band. The (7,7) armchair carbon nanotube is thus a zero-gap semiconductor. Similar as showing Figure (3) that deal with energy dispersion relation for (10,10) armchair carbon nanotubes.



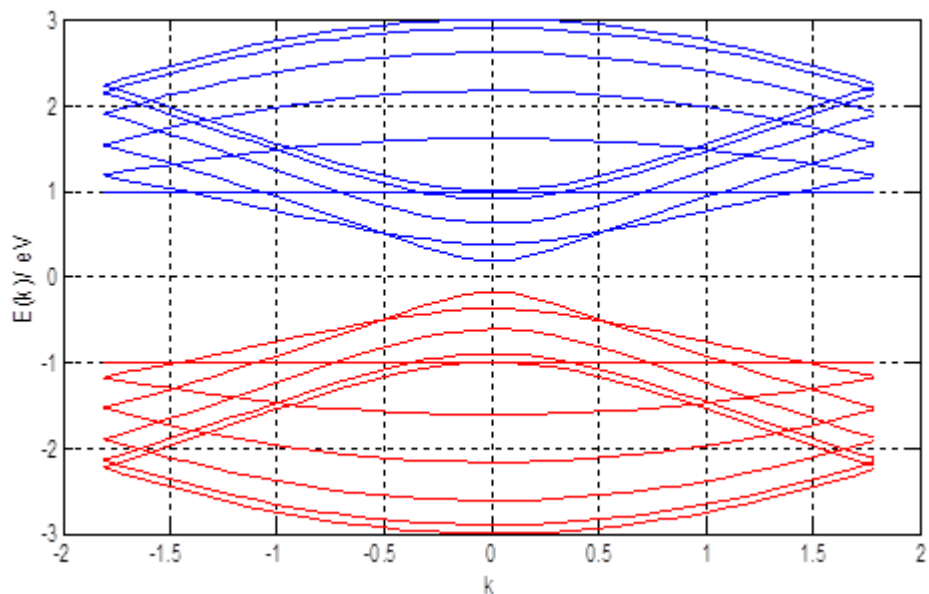
**Figure (3) One-dimensional energy dispersion relations for armchair (10,10) carbon nanotube.**

For the case of energy dispersion relations for zigzag carbon nanotube of (7,0) in Figure(4), the number of valence and conduction bands is 8, with 2 nondegenerate levels and 6 double degenerate levels yielding a total of 14 states, as expected from the number of hexagons for a circumferential ring in the 2D honeycomb lattice. Most important is the band degeneracy that occurs at  $k = 0$  between the doubly degenerate valence and conduction bands.



**Figure(4) One-dimensional energy dispersion relations for zigzag (7,0) carbon nanotube.**

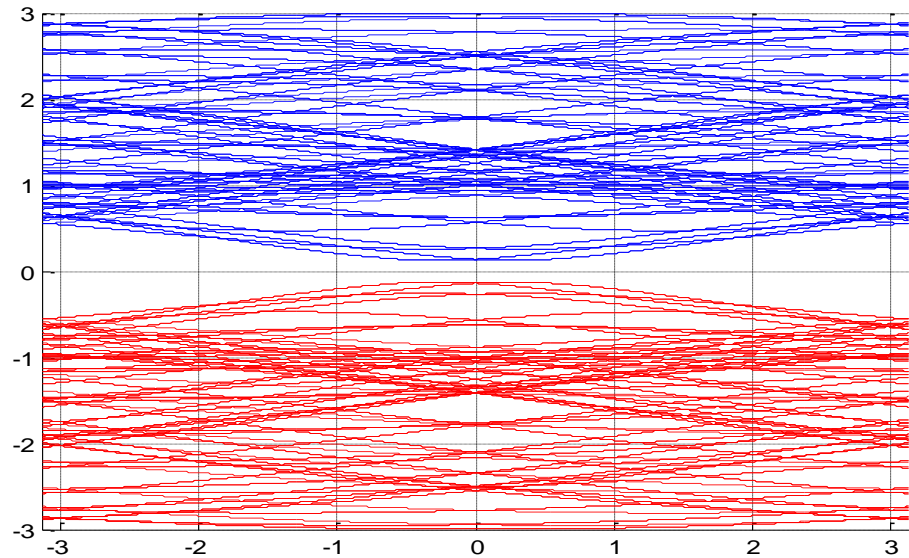
Figure (5) show the illustrative purposes the normalized energy dispersion relations for zigzag (10,0).



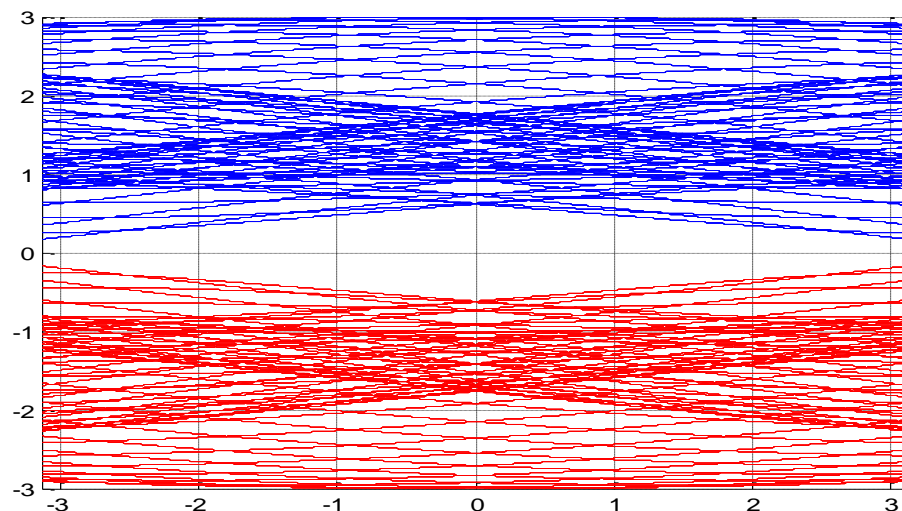
**Figure(5) One-dimensional energy dispersion relations for zigzag (10,0) carbon nanotube.**

For the third type of CNT which is achiral of the energy dispersion relation was calculated by taking the range of  $ka_0 = -\pi: \pi$ . The energy dispersion relation for (10,5) shown in fig.(6) have 70 energy band and for (20,5) that shown in Figure (7) is also have 70 energy band because (10,5) is semiconductor carbon nanotube (i.e  $n-m \neq 3d_R$ ) and (20,5) is metal carbon nanotube (i.e  $n-m = 3d_R$ ). So the number of energy dispersion relation of any chiral is  $N-1$ , where  $N$  is the number of hexagons/cell.

$$N = \frac{2(m^2 + n^2 + nm)}{d_R} \quad \dots(12)$$



**Figure(6) One-dimensional energy dispersion relations for chiral (10,5) carbon nanotube.**



**Figure(7) One-dimensional energy dispersion relations for chiral (20,5) carbon nanotube.**

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