Theoretical Description for Zitterbewegung of electrons in SWCNT (Single Wall Carbon Nanotubes)

The 5th International Scientific Conference for Nanotechnology and Advanced Materials and Their Applications ICNAMA 2015 (3-4Nov.2015

Dr. M. J. Majid
College of Education ,University of Basrah / Basrah .
Email: majid_alsamer@yahoo.com
Dr. S. S. Savinskii
Udmurt State University, Izhevsk , Udmurtia , Russian Federation

Abstract

   The problem of the time evolution of localized quantum states for electrons in the semiconducting and metallic single wall carbon nanotubes (SWCNT) are studied analytically and numerically. In the long-wave approximation $a k_0 \leq 1$, where a is the interatomic distance of carbon atoms in the graphene lattice, k_0 the carrier wave vector of the wave packet, we consider the time evolution of localized quantum states by using a model Hamiltonian. The localized quantum states are interpreted as a superposition of the valence band and the conduction band. The dynamic of the wave packet which is represented by localized quantum states in carbon nanotubes was considered with cylindrical symmetry. The time dependent average values of the angular and axial coordinate operators and its oscillations behavior are calculated. In addition, we taken into account the effect of an external magnetic field which is applied along the axis of carbon nanotube. The evaluations of the frequency and amplitude of zitterbewegung in the carbon nanotube are presented, which can be used for the experimental prospective studies in the nanoelectronic applications.

   Heisenberg representation in the present study are used to evaluate the average values of the coordinate operators , furthermore , Schrödinger representation are used for interpreting the results of the trembling motion (Zitterbewegung) in the carbon nanotubes.

Keywords: Carbon Nanotubes, Zitterbewegung, Localized Quantum States, Wave Packets.

الوصف النظري لظاهرة الزتربيويكنك للالكترونات في الانابيب النانويه الكاربونيه الاحادية الجدار

الخلاصة

تمت في هذا البحث دراسه مسألة النمو الزمني للحالات الكميه المتموقعه للالكترونات في الانابيب النانويه الكاربونيه الاحادية الجدار شبه الموصله والموصله وحلها تحليليا وعدديا. وقد تم استخدام نموذج للمؤثر الهاملتوني في تقريب الموجه الطويله $a k_0 \leq 1$ حيث ان a تمثل المسافه بين ذرات الكاربون في شبيكة الكرافين، k_0 متجه الموجه الحامل بحزمة الموجه، ان الحالات الكميه المتموقعه فسرت على انها عباره عن تراكب او تداخل ما بين حزمة التكافؤ وحزمة التوصيل. الديناميكيه الحركيه لحزمة الموجه والممثله بالحالات الكميه المتموقعه في الانابيب النانويه الكاربونيه تم اعتبارها على انها ذات تماثل اسطواني. تضمن البحث دراسة معدل القيمه لمؤثر الموقع الزاوي والمحوري (الطولي)

والمعتمد على الزمن لكلا النوعين من الانابيب النانويه الكاربونيه. بالاضافه الى ذلك، تم الاخذ بنظر الاعتبار تأثير تسليط مجال مغناطيسي على طول محور الانبوب النانوي الكاربوني. وقد تضمنت نتائج الدراسه تقييم كل من التردد والسعه للحركه الارتعاديه (الزتربيويكنك) للالكترونات في الانابيب النانويه الكاربونيه، والتي قد تسهم في تطور الدراسات المستقبلية التجريبية في مجال الألكترونيات النانويه. في دراستنا الحاليه تم الاعتماد على تمثيل هايزنبرك لغرض حساب معدل القيمه لمؤثر الموقع بالاضافه الى انه تم الاستعانه بتمثيل شرودنكر لغرض تفسير نتائج الحركه الارتعاديه للالكترونات في الانابيب النانويه الكاربونيه قيد الدراسة.

الكلمات المرشدة : الانابيب النانويه الكاربونيه، الظاهرة الارتعاديه،الحالات الكميه المتموقعه،الحزم الموجيه.

INTRODUCTION

It is known from theoretical studies of localized quantum states of a free electron, which is represent a solutions to the one particle relativistic Dirac equation, gives rise to phenomena associated with the concept of Zitterbewegung (ZBW, literally, "jitter", see, e.g., [1]), which occur at a relatively low spatial scales of about Compton wavelength and small time scales inversely proportional to the magnitude of the energy gap $\Delta t \approx \hbar /(2mc^2) \approx 10^{-21} \sec$, m is the mass of electron, c is the speed of light in vacuum, and $\hbar$ is the reduced Planck's constant).

At first, the (Zitterbewegung) or trembling motion of electrons, is devised by Schrödinger for free relativistic electrons in a vacuum [2], has become in the last two years subject of great theoretical studies as it has turned out that this phenomenon should occur in many situations in semiconductors. This problem for the localized electron quantum states having a cylindrical symmetry in the semiconductor carbon nanotube was analyzed in Ref.[2]. In addition to that, we examined the general problem of the time evolution of localized quantum state for metallic and semiconducting carbon nanotube.

The interference of quantum states in the valence and conducting bands of the electronic spectrum lead to emergence of fluctuation (oscillation) in the average values of the coordinates and velocities of electrons as known a phenomenon of Zitterbewegung (ZBW), Many theoretical studies are applied to the two-dimensional semiconducting structures such us graphene (see. review [2]). The similarity of ZBW phenomena in graphene and carbon nanotube associated with the peculiarities of the electronic spectrum and inheriting of the electronic properties of carbon nanotubes from the electronic properties of graphene [3]. The fact of inheriting of the electronic properties has a geometrical interpretation: the carbon nanotube can be represented as a folding of the graphene sheet. Difference of ZBW phenomena in carbon nanotubes and graphene due to the quantization of the transversal component of the electron momentum under folding of the graphene sheet, well as different dimensions: graphene represent as a two dimensional structure, carbon nanotubes - quasi-one dimensional structure [4].

Theoretical Formulation

In the long-wave length limit, Hamiltonian operator of the electron in the carbon nanotube is derived from the Hamiltonian of graphene which is described its band structure as follows [5]:

$$H = V_F (\sigma_x p_x + \sigma_y p_y) \qquad \qquad \dots (1)$$

where $V_F = 1 \times 10^8 \, cm/s$ - is the carrier velocity , p_x, p_y - are the components of the momentum operator, σ_x, σ_y – Pauli matrices. The eigen functions of the Hamiltonian are plane waves. Let us consider the equation of the time evolution of the coordinate (position) operators in Heisenberg representation for the Hamiltonian in equation (1) , using the following relations:

$$-i\hbar \, \dot{x}(t) = [H, x(t)] \quad , \quad -i\hbar \, \dot{y}(t) = [H, y(t)] \quad , \qquad \qquad \dots (2)$$

where $x(t), y(t)$ are the coordinate operators, $\hbar$ - the reduce Planck's constant, the square brackets denote to the commutation of operators. By calculating the right part of equation (2), and taking into account the commutation relations between the momentum and coordinate operators $[p_x, x(t)] = -i\hbar$, $[p_y, y(t)] = -i\hbar$, which leads to the following equations of evolution :

$$-i\hbar \, \dot{x}(t) = -i\hbar \, \sigma_x(t) V_F \; ; \; -i\hbar \, \dot{y}(t) = -i\hbar \, \sigma_y(t) V_F \; ;$$

$$-i\hbar \, \dot{\sigma}_x(t) = [H, \sigma_x(t)] \; ; \; -i\hbar \, \dot{\sigma}_y(t) = [H, \sigma_y(t)] \quad , \qquad \qquad \dots (3)$$

where $\sigma_x(t), \sigma_y(t)$ - Heisenberg operators which are corresponds at the initial (zero) time to Pauli matrices $\sigma_x(0), \sigma_y(0)$ respectively . By integrating the equations (3) and rearranging the terms, we would have obtain the following operators of time dependent coordinate [6] :

$$x(t) = x(0) + \frac{V_F^2 \, p_x t}{H} + \frac{i\hbar V_F}{2} \left(\sigma_x(0) - \frac{V_F p_x}{H} \right) \frac{1}{H} \left(\exp(-2iHt/\hbar) - 1 \right)$$

$$y(t) = y(0) + \frac{V_F^2 \, p_y t}{H} + \frac{i\hbar V_F}{2} \left(\sigma_y(0) - \frac{V_F p_y}{H} \right) \frac{1}{H} \left(\exp(-2iHt/\hbar) - 1 \right) \quad , \qquad \dots (4)$$

where $x(0)$, $y(0)$ – the initial values of coordinates, $\dfrac{1}{H}$ - the inverse Hamiltonian operator. Its clear form formula (4) that it's includes linear dependence with time and oscillating behavior in third terms, which is responsible for the phenomenon of zitterbewegung (ZBW).

By Differentiating the equation (4) with respect to time ,may be can to obtain Heisenberg operators for projection of the electron velocity and current. Consider the geometrical procedure for obtaining a carbon nanotube by rolling graphene sheet, leading to a change in the electronic spectrum. The transformation of the electronic spectrum in the graphene by folding the sheet can be understood from the following considerations: for the Hamiltonian (1), we consider the eigen functions which are represent a plane wave that correspond to the periodicity conditions at opposite ends of graphene sheet in the direction of the axis Ox. This condition leads to the following eigen function [7]:

$$\left| \psi_{k_y n S} \right\rangle = \frac{1}{\sqrt{BL}} \exp \left(ik_x(n) x + ik_y \, y \right) \frac{1}{\sqrt{2}} \begin{pmatrix} b\,(n, k_y) \\ S \end{pmatrix} , \quad b\,(n, k_y) = \frac{k_x(n) - i k_y}{\sqrt{k_x^2(n) + k_y^2}}, \qquad \dots (5)$$

where $k_{\varphi x}(n) = \dfrac{2\pi}{L} \left(m + \varphi - \dfrac{v}{3} \right)$ is the discrete component of the projection of the wave vector on the axis Ox, n :the number of discrete quantum states in the band ; L - the width of the graphene sheet in the direction of the axis Ox, *B* is the length of the

Eng. &Tech.Journal, Vol.33, Part (B), No.5 2015   **Theoretical Description for Zitterbewegung of**
electrons in SWCNT (Single Wall Carbon
Nanotubes)

strip in the direction of the axis Oy ; v is an integer ($v= 0$ or ± 1) determined by the structure. Metallic and semiconducting nanotubes correspond to $v= 0$ and $v=\pm 1$, respectively ; φ with ϕ being a magnetic flux passing through the cross section and ϕ_o being the flux quantum given by $\phi_o = ch/e$. The wave function (5) represent a two-pseudospinors , each component of pseudospinors defines the coordinate wave function of an electron localized on one of the two atomic sublattices of the graphene sheet (A and B sublattice). In the formula (5) parameter S = ± 1 enumerates the positive and negative branches of the energy $E_{k_y nS} = S V_F \hbar \sqrt{k_x^2(n) + k_y^2}$, $\hbar k_y$ - the electron momentum along the axis Oy.

The above formula (5) allow us to identify the wave functions and energies of the electronic states on the surface of carbon nanotubes in the long-wave approximation, to achieve this procedure we make the change in variables, let us assume a new notation: $x \rightarrow R\varphi, y \rightarrow z$, $L = 2\pi R$, where R :the radius of the nanotube, $0 \le \varphi \le 2\pi$ - polar coordinates. As a result, the wave functions (5) defined on the graphene sheet in cylindrical coordinates on the surface of the carbon nanotubes can be summarized as follows:

$$\left| \psi_{kmS} \right\rangle = \frac{1}{2\pi\sqrt{R}} \exp(im\varphi + ik z)\frac{1}{\sqrt{2}} \begin{pmatrix} b(m,k) \\ S \end{pmatrix}, \quad b(m,k) = \frac{k_\varphi(m) - ik}{\sqrt{k_\varphi^2(m) + k^2}}, \qquad \dots(6)$$

$$E_{kmS} = S V_F \hbar \sqrt{k_\varphi^2(m) + k^2} ,$$

$k_\varphi(m) = \frac{1}{R}\left(m + \varphi - \frac{v}{3} \right), \quad m = 0, \pm 1, \pm 2,\dots.$ magnetic quantum number , inherited from quantum number n that used in the formula (5), the wave vector k is derived from the wave vector components k_y. It should be noted the wave function (6) constructed from (5), is a two-pseudospinors components which determine the wave functions of the electrons localized on the two sublattices of the carbon nanotubes. The normalization condition for the function (6) has the form:

$$\left\langle \psi_{kmS} \middle| \psi_{k'm'S'} \right\rangle = \delta(k - k') \, \delta_{mm'} \, \delta_{SS'} , \qquad \dots(7)$$

where the right side is the product of the Dirac delta function and Kronecker symbols, the integration in (7) is over an infinite cylindrical surface of radius R. The normalization factor of the wave function (6) can be formally obtained from the formula (5), considered the limit $B \rightarrow \infty$.

The quantum state (6) is a localized wave on a cylindrical surface. The value of $\hbar k$ in a quantum state determines the momentum of the electron along the cylinder, the magnetic quantum number m determines the angular momentum of the electron. Consider an arbitrary quantum state in the initial (zero) time for an electron on a carbon nanotube, which is represented as a superposition of eigen functions (6):

$$\left| \psi(0) \right\rangle = \sum_{m,S} \int_{-\infty}^{\infty} a_{kmS} \left| \psi_{kmS} \right\rangle dk , \quad a_{kmS} = \left\langle \psi_{kmS} \middle| \psi(0) \right\rangle. \qquad \dots(8)$$

The average value of the cylindrical coordinates for the quantum state (8) at an arbitrary time can be calculated using the above formula for the coordinate operators in Heisenberg representation: The operators $\varphi(t)$, $z(t)$ are determined from

formulas (4) by change the notation of Heisenberg coordinates $x(t) \rightarrow R\varphi(t)$, $y(t) \rightarrow z(t)$ and replacing the momentum operators $p_x \rightarrow -i\hbar \frac{1}{R}\frac{\partial}{\partial \varphi}, p_y \rightarrow -i\hbar \frac{\partial}{\partial z}$. The formulas for calculating the average values of the cylindrical coordinates operators are given as follows:

$$R\overline{\varphi}(t) = \langle \psi(0)| R\varphi(t)\rangle |\psi(0)\rangle, \overline{z}(t) = \langle \psi(0)|z(t)\rangle |\psi(0)\rangle, \qquad \dots (9)$$

by taking into account the representations for the function $|\psi(0)\rangle$ (8), including the matrix elements $\langle \psi_{kmS}|R\varphi(t)|\psi_{k'm'S'}\rangle$ and $\langle \psi_{kmS}|z(t)|\psi_{k'm'S'}\rangle$. The integration of spatial cylindrical variable in a given matrix elements, taking into account (6) leads to a factor that is equal to the product of the Dirac delta function and Kronecker delta $\delta(k-k') \, \delta_{mm'}$, the summation on the index m' leads to the following formulas :

$$R\overline{\varphi}(t) = \sum_{m=-\infty}^{\infty} \sum_{S,S'=\pm 1} \int\int_{-\infty-\infty}^{\infty\,\infty} a_{kmS}^* \, a_{k'mS'} \langle \psi_{kmS}|R\varphi(t)|\psi_{k'mS'}\rangle \, dk\,dk',$$

$$\overline{z}(t) = \sum_{m=-\infty}^{\infty} \sum_{S,S'=\pm 1} \int\int_{-\infty-\infty}^{\infty\,\infty} a_{kmS}^* \, a_{k'mS'} \langle \psi_{kmS}|z(t)|\psi_{k'mS'}\rangle \, dk\,dk'. \qquad \dots(10)$$

The non-zero matrix elements of the coordinates are computed by using the formulas (4) and (6) in Heisenberg representation:

$$\langle \psi_{km+1}|R\varphi(t)|\psi_{k'm+1}\rangle = -\langle \psi_{km-1}|R\varphi(t)|\psi_{k'm-1}\rangle = \frac{V_F k_\varphi(m)t}{\sqrt{k_\varphi^2(m)+k^2}}\delta(k-k') \ ,$$

$$\langle \psi_{km+1}|R\varphi(t)|\psi_{k'm-1}\rangle = \langle \psi_{k'm-1}|R\varphi(t)|\psi_{km+1}\rangle^* = -\frac{1}{2}\left(\frac{k}{k_\varphi^2(m)+k^2}\right)\times$$
$$\left(\exp(+2iV_F\sqrt{k_\varphi^2(m)+k^2}\,t)-1\right)\delta(k-k');$$

$$\langle \psi_{km+1}|z(t)|\psi_{k'm+1}\rangle = -\langle \psi_{km-1}|z(t)|\psi_{k'm-1}\rangle = \frac{V_F k t}{\sqrt{k_\varphi^2(m)+k^2}}\,\delta(k-k') \ ,$$

$$\langle \psi_{km+1}|z(t)|\psi_{k'm-1}\rangle = \langle \psi_{k'm-1}|z(t)|\psi_{km+1}\rangle^* = \frac{1}{2}\left(\frac{k_\varphi(m)}{k_\varphi^2(m)+k^2}\right)\times$$
$$\left(\exp(+2iV_F\sqrt{k_\varphi^2(m)+k^2}\,t)-1\right)\delta(k-k').$$

$$\dots(11)$$

We note that, in the formulas (11) the values of matrix elements at zero time are assumed to equal zero. To calculate the wave function and electronic density distribution on the cylindrical surface at any given time for the quantum state mentioned above, is necessary to use Schrodinger representation for the wave function of a quantum state:

$$\left|\psi(t)\right\rangle = \exp(-iHt/\hbar)\left|\psi(0)\right\rangle,$$

by using the formula (8) we have:

$$\left|\psi(t)\right\rangle = \sum_{m,S} \int_{-\infty}^{\infty} \exp(-\frac{i}{\hbar}E_{kmS}\,t)\,a_{kmS}\left|\psi_{kmS}\right\rangle \quad . \qquad \ldots(12)$$

Let us consider a localized electronic states which represent at zero time a wave packet centered on the surface of the carbon nanotubes ,where the angle $\overline{\varphi}(0) = \pi$ and coordinates $\overline{z}(0) = 0$, [8] :

$$\left|\psi(0)\right\rangle = A\exp(-\frac{z^2}{2d^2}+ik_0z)\exp(-\frac{(\varphi-\pi)^2}{2\sigma^2}+im_0\varphi)\binom{\alpha}{\beta},$$

$$A = \frac{1}{\sqrt{|\alpha|^2+|\beta|^2}\sqrt{\pi\,dR\,\sigma\,erf\left(\frac{\pi}{\sigma}\right)}}, \qquad \ldots (13)$$

where d - define the localization size of the packet for axial coordinate parameter and σ – localization extension of the packet over the angular variable, k_0 - the carrier wave vector , m_0 - the magnetic quantum number. The parameters α and β defines the relation between the components of the pseudospin function. The expansion coefficients of the wave function (13) in the eigen functions (6) $a_{kmS} = \left\langle\psi_{kmS}\left|\psi(0)\right\rangle$ yield the following formula [8]:

$$a_{kmS} = \frac{A\,d\,\sigma\sqrt{R}}{2\sqrt{2}}\left(\alpha\,b_0^*(m,k)+\beta\,S\right)\exp\left(-\frac{(k-k_0)^2d^2}{2}\right)$$

$$\exp\left(i\pi(m_o-m)-\frac{\sigma^2}{2}(m-m_0)^2\right) \qquad \ldots (14)$$

$$\left(erf\left(\frac{\pi+i\sigma^2(m_0-m)}{\sqrt{2}\sigma}\right)+erf\left(\frac{\pi-i\sigma^2(m_0-m)}{\sqrt{2}\sigma}\right)\right)$$

Where $erf(\cdots)$ - Laplace function [9].

As refer from equation (13), for any parameters α and β there are available states with positive and negative energy (for values (i.e. parameter $S = \pm1$).

$$\overline{x}(\tau) = \frac{d\sigma}{16\pi^3\,erf\left(\frac{\pi}{\sigma}\right)}\sum_{m=-\infty}^{\infty}\left(erf\left(\frac{\pi+i\sigma^2(m_o-m')}{\sqrt{2}\sigma}\right)+erf\left(\frac{\pi-i\sigma^2(m_o-m')}{\sqrt{2}\sigma}\right)\right)^2$$

$$\exp\left(-\sigma^2(m_o-m')^2\right)\int_{-\infty}^{\infty}\exp\left(-(q-q_o)^2\frac{d^2}{R^2}\right)\left(\frac{-q}{(m'+q^2)}\right) \qquad \ldots (15)$$

$$\left(\cos(2\tau\sqrt{m'+q^2})-1\right)dq$$

$$\bar{y}(t) = \frac{d\sigma}{16\pi^3\, erf\left(\frac{\pi}{\sigma}\right)} \sum_{m=-\infty}^{\infty} \left(erf\left(\frac{\pi + i\sigma^2(m_o - m')}{\sqrt{2}\sigma}\right) + erf\left(\frac{\pi - i\sigma^2(m_o - m')}{\sqrt{2}\sigma}\right) \right)^2$$

$$\exp\left(-\sigma^2(m_o - m')^2\right) \int_{-\infty}^{\infty} \exp\left(-(q-q_o)^2 \frac{d^2}{R^2}\right) \left(\frac{m'}{(m'+q^2)}\right) \qquad \dots (16)$$

$$\left(\cos(2\tau\sqrt{m'+q^2}) - 1 \right) dq$$

For large time intervals, each of localized quantum states with positive and negative energy split into two independent sub wave packet(subpacket). The velocities of these subpackets along the cylindrical axis is defined through the group velocities which are calculated for $k = k_0$, $m = m_0$ as following :

$$V_{zp} = \frac{1}{\hbar} \frac{\partial E_{km_0 S}}{\partial k}\bigg|_{k=k_0} = \frac{S V_F k_0}{\sqrt{k_\varphi^2(m_0) + k_0^2}} \quad , \qquad \dots (17)$$

a sign of the group velocity is determined by the value of parameter S. The angular velocity of the rotational motion of the wave packet along the cylindrical surface can be roughly estimated by the formula:

$$R\Omega \approx \frac{S V_F k_\varphi(m_0)}{\sqrt{k_\varphi^2(m_0) + k_0^2}} \,, \qquad \dots (18)$$

where Ω - angular velocity of rotational motion. It was shown that, indeed, the two wave packets represented by the quantum state (13), rotates separately on each other in time at the cylindrical surface of the nanotubes in the direction determined by the sign of the parameter S, the trajectory of a single wave packet can be represented as a helical (spiral) line on a cylindrical surface.

Let us consider localized quantum state, which can be regarded as a special case for the parameter $\sigma \to \infty$ in the formula (13)

$$|\psi(0)\rangle = A \exp\left(-\frac{z^2}{2d^2} + i k_0 z + i m_0 \varphi\right) \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, A = \frac{1}{\sqrt{|\alpha|^2 + |\beta|^2}\sqrt{2\pi\sqrt{\pi}\, dR}}, \qquad \dots (19)$$

the coefficients $a_{kmS} = \langle \psi_{kmS} | \psi(0) \rangle$ can be easily calculated for the non-zero coefficient a_{kmS} at the value of the quantum number $m = m_0$.

$$a_{km_0 S} = A d \sqrt{R}\sqrt{\pi} \left(\alpha\, b_0^*(m_0, k) + \beta\, S\right) \exp\left(-\frac{(k-k_0)^2 d^2}{2}\right)$$

Results, Discussion and Conclusions

The considered localized quantum states are represented by a Gaussian wave packet, which including the positive energies (S = + 1), and negative energies (S = -1) as mentioned above in eq.6. In present study ,we note that for each of the solitary wave packets, the average value coordinate $\bar{z}(t)$ which are calculated by the

formulas (10) and (11), must be taking into account only the diagonal matrix element for z- coordinates, according to above representation ,we obtained the linear time dependence for the average value coordinate $\bar{z}(t) = \overline{V}_z t$, including an average velocity over all quantum states $\overline{V}_z$, which coincides with the group velocity for motion of the wave packet along the axis of the cylindrical structure of carbon nanotube (eq. 17). Analogous conclusions for the wave packet, it's possible by considering the diagonal matrix element of the coordinate operator φ in the evaluation of the average $\overline{\varphi}(t)$,that lead to linear dependence $\overline{\varphi}(t) = \overline{\Omega} t$, includes the angular velocity of rotation $\overline{\Omega}$,which can be approximately calculated by the formula 18.

In Special case of the choice of parameters α, β was considered for localized quantum state (eq. 13), as an example, we consider the case $\alpha = 1; \beta = 0$, which represents at the initial time a localized quantum state on the atomic sublattice A of graphene. This quantum state will be spread with time onto the two sublattices A and B.

Fig. 1 shows the time dependent average value of the axial coordinates of localized quantum state $\alpha = 1; \beta = 0$,for semiconducting carbon nanotube (i.e. *v*= ±1).

In our numerical calculations for the average values , the dimensionless variables are considered: the wave vector $Q = q R$, carrier wave vector $Q_0 = q_0 R$, $\dfrac{d}{R}$ dimensionless parameter of quantum state localization along the axis of the cylinder (Carbon nanotube). Fig.1-a, shows the time dependent average value of the coordinates $\bar{z}(t)$ for magnetic quantum number *m* = 0, in the absence of the external magnetic field (i.e. ϕ=0) . The oscillating behavior disappear or decrease with time and there remains a shift which is related to amplitude of the average value of the coordinates $\bar{z}(t)$ (eq.16) .Our results are coincide with other studies in the computation of the average value of the axial coordinate for semiconducting carbon nanotubes (see Ref.[4]).

By applying an external magnetic field along the axis of nanotube *z*, i.e., in the presence of a magnetic flux ϕ passing through the cross section [8], the flux leads to the change in the boundary condition $\Psi(r + L) = \Psi(r) \exp(+2\pi i \varphi)$ where: $\varphi = \phi / \phi_o$

Fig.1-b and c gives an illustration the effect of the external magnetic field to the behavior of the Zitterbewegung phenomenon in the semiconducting carbon nanotubes for subband *v*=1 (conduction band) for different values of magnetic flux ϕ . It's clear that for small values of magnetic flux ,zitterbewegung oscillation exhibit an decreasing , on the other hand , the amplitude of the average value coordinate increased and the disappearance of oscillations be faster (see fig.1-b). Consequently, the effect of increasing in the value of magnetic flux appear in fig.1-c appear in the excess at the oscillating behavior and the opposite direction of the average value coordinate $\bar{z}(t)$ for magnetic flux ϕ =1.That leads to the opposite orientation in the subpacket motion along the axis of carbon nanotube.

Thus, the transient character of the zitterbewegung oscillations is decrease due to the increasing spatial separation of the subpackets for the general wave packet

which is splits into two parts of subpackets corresponding to the positive and negative energy states (S=±1).
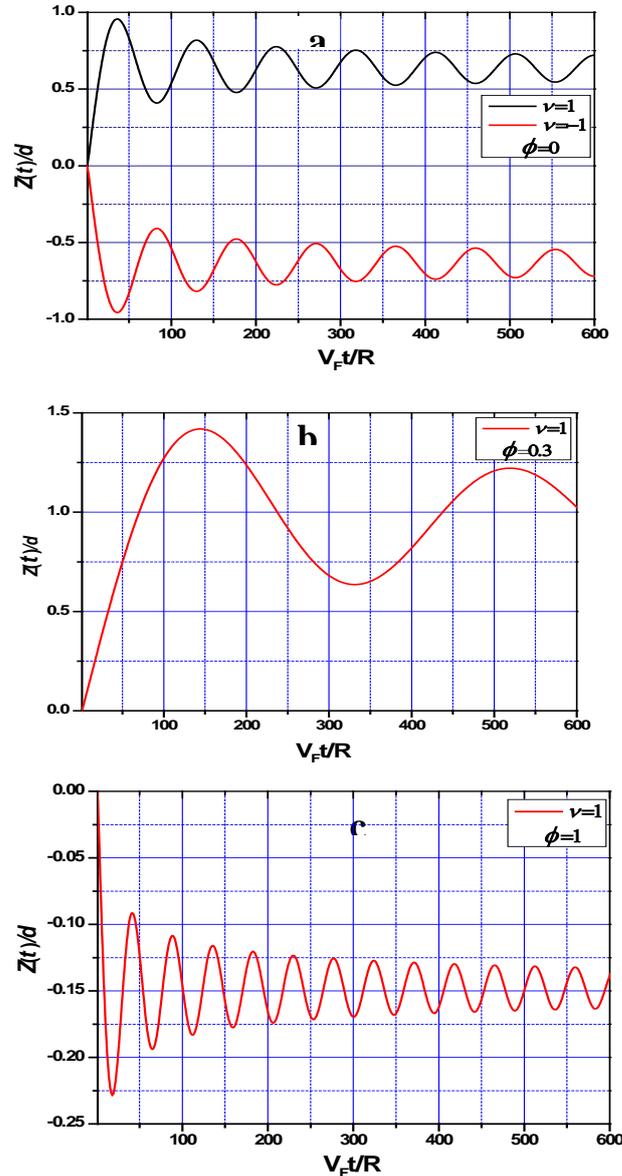
Figure (1) - The time dependent average value of the axial coordinates for semiconducting carbon nano tubes with localized quantum state $\alpha = 1; \beta = 0$

Coordinates for parameters $\alpha = 1, \beta = i$. It's clear that the transient zitterbewegung decrease in the amplitude of an oscillation. The modulation of the damped oscillations associated with the rotation of the two parts of wave packets in opposite direction along the surface of a carbon nanotube. Fig.2 –c,d demonstrate the behavior of the time dependent average values for metallic carbon nanotube in the presence of a magnetic flux, comparably, as mentioned above, the transient zitterbewegung oscillations increase slightly for angular and axial coordinates.

The oscillation of time dependent average values coordinate associated with non-diagonal matrix elements of the coordinate operators, the characteristic frequency for the localized quantum state can be estimated by the following formula:

$$\omega^{ZB} \approx 2V_F \sqrt{q_\varphi^2(m_0) + q_0^2}$$

Accordingly, the characteristic spatial scale of these oscillations for axial and angular coordinates can also be estimated from the term responsible for the zitterbewegung of the non-diagonal matrix elements, as follows [10]:

$$\frac{\Delta z^{ZB}}{d} \approx \frac{R}{d}\left(\frac{m_0}{m_0^2 + Q_0^2}\right) \quad , \quad \Delta\varphi^{ZB} \approx \frac{Q_0}{m_0^2 + Q_0^2} \quad .$$

As mentioned above, the oscillation dependence in all cases can be described as a damped behavior, the damping times can be estimated by the characteristics of kinematic motion of the wave packets:

$$\Delta t_z^{ZB} \approx \frac{d\sqrt{q_\varphi^2(m_0) + q_0^2}}{V_F\, q_0} \quad , \quad \Delta t_\varphi^{ZB} \approx \frac{R\sigma\sqrt{q_\varphi^2(m_0) + q_0^2}}{V_F\, q_\varphi(m_0)}$$
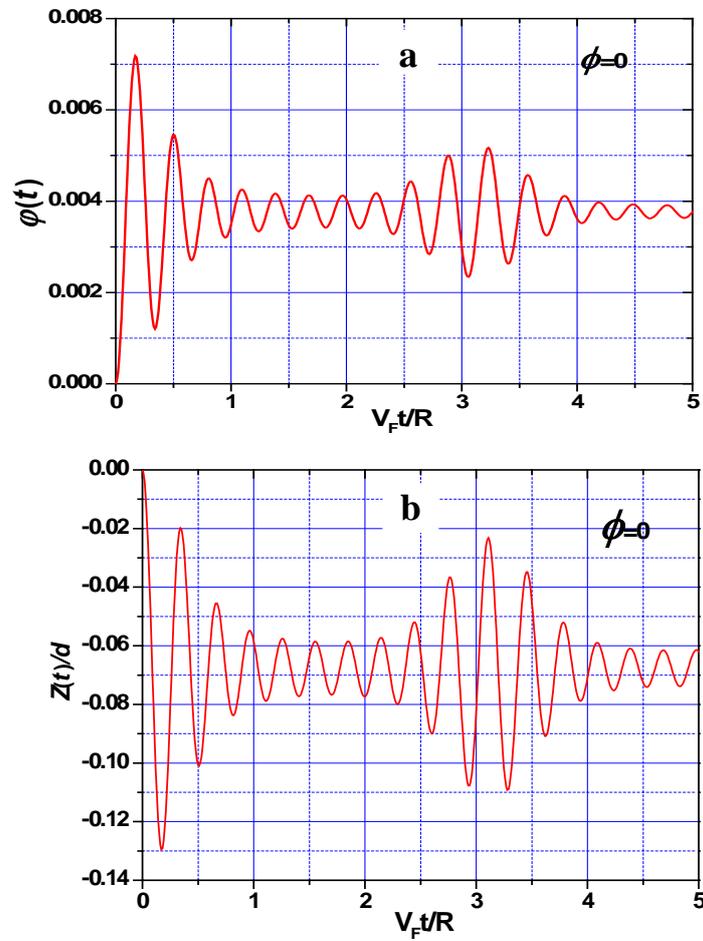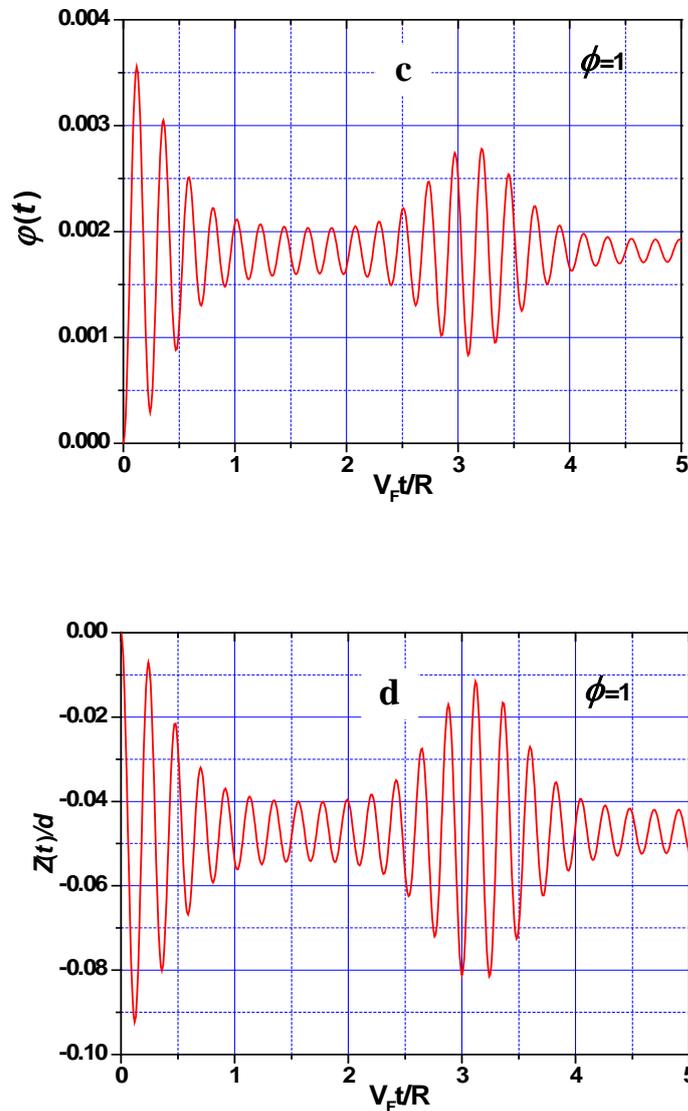
Figure (2) The time dependent average value of axial and angular coordinates for metallic carbon nano tubes with localized quantum state $\alpha = 1; \beta = i$

Thus, our conclusion confirmed that,the possibility of existence the zitterbewegung (ZBW) for localized quantum states of electrons at the surface of the metallic (conductive) and semiconducting carbon nanotube. In view of our results it is clear that, in order to observe the transient zitterbewegung, it is necessary to achieve a superposition between two branches of energy states(positive and negative states S=±1).

References

[1] Itzykson C. and Zuber J. B., Introduction to Quantum Field Theory, McGraw_Hill, New York, vol.1,1980.

[2] Rusin T.M., Zawadzki W., "Zitterbewegung (Trembling Motion) of Electrons In Semiconductors: A Review", J. Phys.: Condens. Matter,Vol.23, P.143201, 2011.

[3] Leonard F. , The Physics Of Carbon Nanotube Devices ,William Andrew Inc. Norwich,NY,USA, P.310 , 2009.

[4] Rusin T.M., Zawadzki W. ,"Transient Zitterbewegung of charge carriers in mono- and bilayer graphene, and carbon nanotubes", Phys.Rev.B.,Vol.76., P.195439, 2007.

[5] Majid M.J., Savinskii S. S.," Features of the Time Evolution of Localized Quantum States in Graphene , Semiconductors", Vol. 47, No. 1, P. 141–145, 2013

[6] Majid M.J., Поздеева Ю.С., "Динамика Электронных Волновых Пакетов В Углеродных Нанотрубках", XX международная конференция студентов, аспирантов и молодых ученых «Ломоносов», Р.294-295 , 2013.

[7] Ando T. ,"Theory of Electronic States and Transport in Carbon Nanotubes", J.Phys.Soc.Jpn.Vol.74, P. 777–817, 2005.

[8] Maksimova G. M., Demikhovskii V. Ya., and Frolova E. V., "Wave Packet Dynamics In A Two-Dimensional Electron Gas With Spin Orbit Coupling: Splitting And Zitterbewegung" , Phys. Rev. B 78,P. 235321,2008.

 [9] Диткин В.А., Кармазина Л.Н., Справочник По Специальным Функциям, Наука, Москва ,1979.

[10] Majid M.J., Савинский С.С., "Динамика Электронных Волновых Пакетов В Углеродных Нанотрубках", ФТВД ,Том 23, №.3,Р.4-14, 2013.