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Article

# Effect of the Width of The Single-Layer Graphene Nanoribbon on the Trembling Motion of Dirac Electrons

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Abstract: This work presents a theoretical investigation of the Zitterbewegung (ZBW) phenomenonan intrinsic trembling motion of Dirac electrons- in armchair-type multilayer graphene nanoribbons (AGNRs). Utilizing the long-wavelength approximation and the Heisenberg representation, the study explores the time evolution of the position operator for electrons described by Gaussian wave packets. Key physical parameters, including ribbon width, initial wave vector, and pseudo-spin polarization, are systematically varied to analyze their impact on the characteristics of ZBW oscillations. The results reveal that ZBW is highly sensitive to these factors, with oscillations occurring within ultrashort timescales (~30 femtoseconds). Notably, wider ribbons and broader wave packets lead to reduced oscillation amplitudes. The role of pseudo-spin configuration is found to be crucial in enabling or suppressing the oscillatory behavior. These findings offer deeper insight into the relativistic-like quantum dynamics of electrons in graphene nanostructures and suggest potential implications for future applications in ultrafast nanoelectronics and quantum devices.

**Keywords:** Graphene; Armchair Graphene Nanoribbon; Trembling motion; Wave packet of electrons; ZBW.

#### 1. Introduction

It was in 1930 that Schrodinger made the prediction that free electrons in a vacuum will experience a phenomenon known as Zitterbewegung (ZBW) [1]. Since the Dirac equation's electron velocity operator does not commute with the Hamiltonian, we may say that the electron velocity is not a motion equation constant. The solutions to the Dirac equation for a relativistic electron in free space are what give rise to the term "thumping velocity," which is used to describe the velocity of an electron when there is no effective external field present [1, 2]. In relativistic quantum systems, the wave packet is a distinguishing feature that differentiates it from nonrelativistic quantum systems. The wave packet's location oscillates over time owing to the strong coupling between the pseudo-spin degree of freedom and momentum [3]. This oscillation is a typical feature of relativistic quantum systems. despite the fact that this phenomenon has received a considerable amount of theoretical attention from the point of view of relativistic theory. The time development of the expected values of certain physical observables, such as location, velocity, current, and spin angular momentum, is a manifestation of the oscillatory dynamic that pertains to the center of a free wave packet.

Zitterbewegung motion's signature frequency is defined by the energy difference between the positive and negative states. This frequency is of the order of  $2m_0c^2/\hbar$ , where  $m_0$  is the mass of the electron, c is the velocity of light, and  $\hbar$  is the Planck constant. But oscillation amplitudes are on the order of the Compton wavelength. So, this is equivalent to very high oscillation frequencies with very tiny amplitudes, both of which are inaccessible using the methods of experimentation that are now in use [4]. Graphene, which is a single layer of a honeycomb lattice of carbon atoms with unique electronic characteristics, has been the subject of a recent reexamination of the Zitterbewegung phenomenon. This is because low-energy electrons in graphene function as quasi-

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relativistic particles [5]. Graphene exemplifies a unique system characterized by linear dispersion at low energy, facilitating a bridge between the high-energy domain and the low-energy condensed matter realm. In spite of the fact that graphene has intriguing characteristics, its applications in semiconductor circuits are restricted due to the fact that the energy gap is very narrow.

However, when a two-dimensional sheet of graphene is sliced into a semi-one-dimensional sheet, graphene may be produced. The production of so-called graphene nanoribbons will result from this process. These nanoribbons may be divided into two primary categories: armchair and zigzag. The geometry of the edge along the nanoribbon is what determines this categorization. By using the weak van der Waals forces, it is feasible to organize the various layers of graphene in a manner that allows them to interact with one another. While the Bernal structure (ABABA...) is the most common ordering of graphite layers, other arrangements are conceivable, and are indicated by the composition (ABCABC A...). Because of this arrangement, graphite formations are said to have a defect or distortion in their crystal structure. Graphite has an interlayer distance of about  $h=0.335 \ nm$ , which is much larger than the distance between carbon atoms in a single layer  $a=0.124 \ nm$ . The difference is that this distance is really large.

Due to the fact that the velocity operator does not commute with the Hamiltonian in the systems, the Zitterbewegung phenomenon was thought to be responsible for the minimal conductivity that was seen in the graphene system in the early research. Using the connection between the theory of the energy bands in narrow-gap semiconductors (NGS) and the free Dirac relativistic equation for electrons [6]. Zawadzki et al. conducted research on ZB in NGS in the year 2005. For a free electron, they discovered that the amplitude and frequency of the oscillation were much more favourable than those in a vacuum [7, 8]. At the same time, Schliemann and colleagues have conducted an in-depth investigation of the ZBW of an electron in III-V zinc-blende semiconductor QWs when the SOI was present. The aforementioned discoveries served as the impetus for further theoretical study on the ZBW of electrons in a variety of condensed matter systems [9, 10].

Graphene, graphene nanoribbons, and carbon nanotubes are examples of carbon nanomaterials that possess remarkable physical and chemical characteristics [11], [12], [13], 14]. These qualities have the potential to be used in the development of promising electronic nanotechnologies [15, 16]. It was for the first time that it was emphasised theoretically that the minimum conductivity of graphene may be described in terms of the phenomena ZBW [17]. Consequently, a large number of academics are interested in it. In 2008, researchers looked at how charge carriers changed time evolution and measured their ZBW in semiconducting carbon nanotubes with cylindrical symmetry, monolayer graphene, and bilayer graphene [18]. Ghosh et al. conducted a theoretical investigation of the occurrence of ZBW as well as the advancement of the wave packet over time in zigzag graphene nanoribbon (ZGNR). They highlighted the fact that the connection between the bulk states and edge states has fascinating characteristics, and they also made the observation that the oscillation in position happens along the direction of the wave packet propagation, which is not possible in the infinite graphene sheets and semiconductor nanowires. Majid and Savinskii [19, 20], along with Majid and Alla [21, 22], examined the impact of different pseudospin polarisations on wave-packet dynamics in monolayer graphene, carbon nanotubes, and graphene nanoribbons, focussing on the initial wave function and the ZBW phenomenon. They did this by using the Heisenberg representation. Also, they investigated the phenomenon of ZBW.

In this study, we perform a comprehensive analytical and numerical analysis of the time-dependent behavior of the projected position operator associated with the Zitterbewegung (ZBW) phenomenon in a monolayer armchair graphene nanoribbon. Our theoretical framework employs the long-wavelength approximation in conjunction with the Heisenberg representation to model the quantum dynamics of low-energy Dirac fermions. Specifically, we investigate the evolution of a two-dimensional Gaussian wave packet, focusing on its oscillatory motion as a result of quantum interference between positive and negative energy states. This approach enables precise characterization of the

transient ZBW oscillations and their dependence on structural and electronic parameters intrinsic to MLAGNRs.

#### 2. Materials and Methods

For the long wave model, the following is the effective low energy Hamiltonian of graphene, which is located at the *K* point in the first Brillouin zone:

$$\widehat{H} = V_F(\sigma_x \widehat{p}_x + \sigma_y \widehat{p}_y) \tag{1}$$

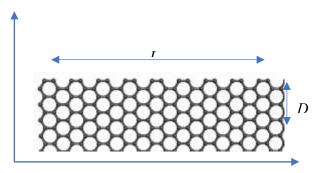
As illustrated in Figure 1, the Fermi velocity is denoted by  $V_F$ , while the Pauli matrices and momentum effects are represented by  $\sigma_x$  and  $\sigma_y$ . Fig. 1depicts the structural diagram of an armchair graphene nanoribbon, which has a length of L and a width of D. On the ribbon, the width is shown as a function of two carbon atoms per unit cell, and it is represented by dashed lines along the y - axis of the ribbon:

$$D = \frac{M}{4}\sqrt{3}a_o \tag{2}$$

where  $a_o$  represents the graphene lattice constant in this formula. Here we can see the energy spectrum of a layered armchair graphene nanoribbon with widths D:

$$E_{ks} = SV_F \hbar \varepsilon , \ \mathcal{E} = \sqrt{1 + 4\cos(k_q)\cos\frac{k}{2} + 4\cos^2k_q}$$
 (3)

where  $k_q = \frac{2}{\sqrt{3}a_0} \frac{q}{M+1} \pi$ , q = 1,2,3,...M,  $S = \pm 1$ .



**Figure 1.** Armchair graphene nanoribbon of length L and width D

It is possible to express the spinor wave function of the Hamiltonian with respect to Eq.2 as follows [23]:

$$\psi_{kqs} = \frac{1}{2\pi\sqrt{DL}} exp(ikx + ik_q y) \frac{1}{\sqrt{2}} {A_k \choose S}, A_k = \frac{k - ik_q}{\sqrt{k^2 + k_q^2}}$$
(4)

where the integer n represents the number of individual quantum states that make up the band. Under the assumption that the graphene nanoribbon is the core of the original wave packet, we may say that it is a superposition of the spinor wave functions. The initial momentum is denoted by  $k_{x0}$ , while the initial momentum is denoted by  $k_{y0}$ :

$$\psi(0) = Bexp\left(-\frac{x^2}{2d^2} - \frac{y^2}{2d^2} + ik_{x0}x + ik_{y0}y\right) {\alpha \choose \beta}$$
 (5)

In our current calculations, the parameters  $\alpha$  and  $\beta$  indicate the polarisation of the pseudo-spin. These parameters provide the connection between the components of the pseudo-spin in the wave function. Additionally, d represents the width of the localised wave packet on the surface of the ribbon. For the wave packet, it is not difficult to get an arbitrary starting quantum state by using the pseudospin's function, as shown in the following:

$$\psi(0) = \sum_{n,s} \int_{-\infty}^{\infty} a_{kns} |\psi_{kns}\rangle, a_{kns} = \langle \psi_{kns} | \psi(0) \rangle$$
 (6)

where  $a_{knS}$  the expansion coefficients of the quantum state are represented.

It is well knowledge that the Heisenberg representation, which may be defined as follows, is responsible for determining the average value of any physical quantity *P* at time t.

$$\langle P(t)\rangle = \langle \psi(0)|\hat{P}(t)|\psi(0)\rangle \tag{7}$$

$$\langle P(t) \rangle = \sum_{s,\bar{s}} \int dk \ a_{ks}^* \ a_{ks} \langle \psi_{ks} | \hat{P}(t) | \psi_{\bar{k}\bar{s}} \rangle \tag{8}$$

In both the longitudinal and transversal directions, the following Heisenberg operators identify the position of the AGNR for the multilayer layers [24, 25]:

$$\hat{x}(t) = \hat{x}(0) + \frac{(V_F)^2 \hat{p}_x}{\hat{H}} t + \frac{iV_F \hbar}{2\hat{H}} \left( \hat{\sigma}_x(0) - \frac{V_F \hat{p}_x}{\hat{H}} \right) \left( e^{-\frac{2iHt}{\hbar}} - 1 \right)$$
(9)

$$\hat{y}(t) = \hat{y}(0) + \frac{(V_F)^2 \hat{p}_y}{H} t + \frac{iV_F \hbar}{2H} \left( \hat{\sigma}_y(0) - \frac{V_F \hat{p}_y}{H} \right) \left( e^{-\frac{2iHt}{\hbar}} - 1 \right)$$
(10)

$$a_{kS}^* a_{kS'} = \frac{d^2}{(|\alpha|^2 + |\beta|^2) 2\pi DL} (\alpha A_k + \beta S) (\alpha A_k^* + \beta S') e^{-(k - k_{X0})^2 d^2} e^{-(k_n - k_{Y0})^2 d^2}$$
(11)

Finally, we arrive at the following formula for calculating the average values of the longitudinal and transversal components of the location of the AGNR for n layers:

$$\langle x(t) \rangle = \sum_{S,S'} \int dk \left\{ \mu(\alpha A_k + \beta S)(\alpha A_k^* + \beta S') \right\} \left\{ \left( \frac{A_k^* A_k + SS'}{2} \right) \left( \frac{V_F k_x t}{S' \varepsilon} \right) + \frac{i}{2S' \varepsilon} \left[ \left( \frac{A_k S + A_k^* S'}{2} \right) - \left( \frac{A_k^* A_k + SS'}{2} \right) \left( \frac{k_x}{S' \varepsilon} \right) \right] \left[ e^{-2iS' V_F \varepsilon t} - 1 \right] \right\}$$
(12)

$$\langle y(t)\rangle = \sum_{S,S'} \int dk \left\{ \mu(\alpha A_k + \beta S)(\alpha A_k^* + \beta S') \right\} \left\{ \left( \frac{A_k^* A_k + SS'}{2} \right) \left( \frac{V_F k_q t}{S' \varepsilon} \right) + \frac{i}{2S' \varepsilon} \left[ \left( \frac{i(A_k S - A_k^* S')}{2} \right) - \left( \frac{A_k^* A_k + SS'}{2} \right) \left( \frac{k_x}{S' \varepsilon} \right) \right] \left[ e^{-2iS' V_F \varepsilon t} - 1 \right] \right\}$$

$$\text{where } \mu = \frac{d^2 Z^2}{(|\alpha|^2 + |\beta|^2) 2\pi DL} e^{-(k - k_{x_0})^2 d^2} e^{-(k_n - k_{y_0})^2 d^2}, Z = \frac{1}{2\pi \sqrt{DL}} \ .$$

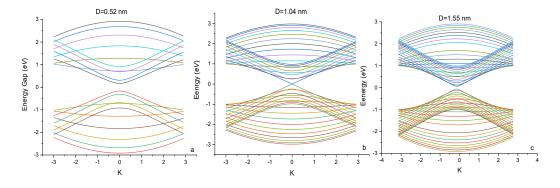
$$(13)$$

#### 3. Results and Discussion

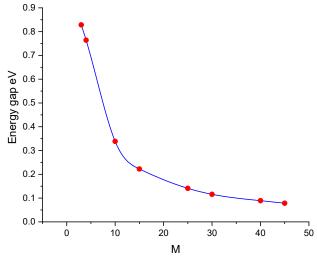
#### 3.1 The band stucture of a single graphene nanoribbon

This section examines the electrical band structure of single-layer graphene nanoribbons, composed of graphene with extensions, and the correlation between the bandgap and their width. This particular graphene nanoribbon has dual characteristics: it functions as both a metallic substance and a semiconductor. Graphene is often recognized as a semiconductor with a zero bandgap; however, its bandgap may be altered by modifying certain characteristics, therefore converting it into a semiconductor with diverse bandgap values.

The bandgap of semiconductors is a crucial attribute that dictates the significance of these materials in nanoelectronics devices, a principal objective of modern technology. Figure 2 illustrates the findings of this study, showing the width of graphene nanoribbons with arms, corresponding to D values of 0.52, 1.04, and 1.55. The conductivity shifts from metallic to semiconducting based on the ribbon width. Upon comparison of Figure 2 (a, b, and c), it is evident that the electrical characteristics of graphene nanoribbons with arms move from metallic to semiconducting features. It is important to observe that when D equals 1.04, the energy gap nears zero, quantitatively measured at  $6.44 \times 10^{-7}$  electron volts. The following graphs vividly illustrate the semiconductor's behaviour via the widening of the energy gap. Figure 3 depicts the correlation between the energy gap and the width of the graphene nanoribbon. It is observed that as the ribbon's width expands, the energy gap values diminish, indicating that the nanoribbon tends towards the metallic behavior characteristic of a graphene sheet.



**Figure 2.** The energy spectrum of a single-layer graphene nanoribbon in the k-space for different values of the width D = 0.52, 1.04, and 1.55 nm.

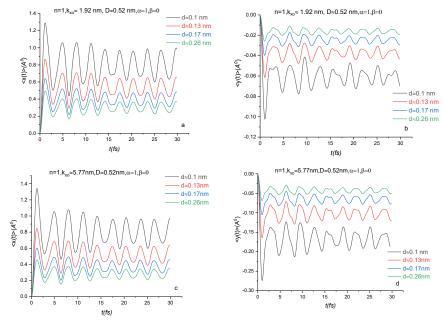


**Figure 3.** Energy gap relationship with the M of a single layer of armchair graphene ribbons.

#### 3.1 ZB phenomenon of single layer graphene nanoribbon

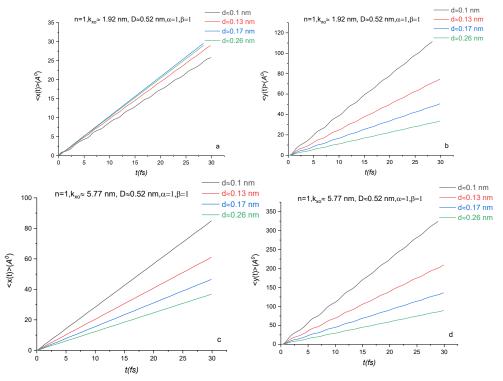
This study offers a theoretical analysis of the Zitterbewegung, sometimes called trembling motion, in armchair graphene nanoribbons with one or more layers. First of several parameters that we set up were the pseudo-polarization coefficients ( $\alpha$  and  $\beta$ ), where  $\alpha$  assumed values of 1 and 0 and  $\beta$  was always 1. Graphene sublattice A or B is more likely to contain the electron at the start of motion, depending on these parameters. Secondly, the x and y directions are taken into account by the initial wave vector k, but the y direction's value,  $k_{y_0} = 0$ , is ignored. The  $k_{x_0}$  takes on different values as a result of quantised motion in the x-direction, but it is calculated using the long-wave model, which connects it with the nanoribbon width (Eq. 2). Third, we tested three different values for D, the nanoribbon's width, at  $0.52 \, nm$ ,  $1.04 \, nm$ , and  $1.55 \, nm$ . A positive integer M, representing the number of lines that correspond to the positions of atoms in the graphene lattice, is necessary for both the initial wave number k and the width of the nanoribbon D. The original unit cell's hexagon after we computed the predictions for x(t) and y(t) as functions of time.

We then used the numerical solutions to equations 12-13 to calculate the expected values of the directions with respect to time, and we displayed this information visually. We calculated the beginning of the trembling motion to be 30 femtoseconds since this phenomenon has a very short lifetime, beginning with the electron's transition between the unit cell's sublattices and the first Brillouin zone, and ending with its decay. As a result, we thought this time value worked well to show the oscillatory motion's increase and decrease in armchair-type graphene nanoribbons. Ribbon length is  $L = 200 \, nm$ , interlayer spacing is  $a = 0.124 \, nm$  in the hexagonal graphene lattice, and the height between layers is  $h = 0.335 \, nm$ . For different values of the Gaussian band width d and starting wave vectors  $k_{y_0} = 0$  and  $k_{x_0} = 1.29, 5.77$  nm. Figure 4 displays the average expected values of the x and y locations with respect to time for a single graphene nanoribbon layer. The figure further demonstrates that the Average expected values oscillate in both directions depending on the nanoribbon width  $D = 0.52 \, nm$ , as the oscillation amplitude is inversely proportional to the wave packet width. We may also see that the oscillation is periodic and regular at these values. Altering the values of the initial wave vector  $k_{x_0}$  did not significantly impact the amplitude or frequency of the oscillation. Zitterbewegung is present in both the transverse and longitudinal directions because the position operators x(t) and y(t) fluctuate.



**Figure 4.** Time-dependent position operator of a single-layer graphene nanoribbon (DD, kk,  $\alpha$ , $\beta\alpha$ , $\beta$ ) showing longitudinal (a, b) and transverse (c, d) oscillations for various Gaussian bandwidths.

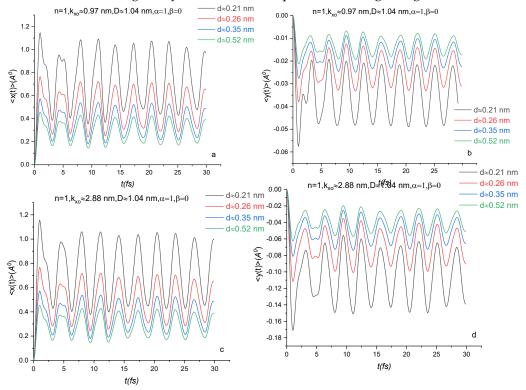
Position operator as a function of time for a single layer of graphene nanoribbon width D=0.52 nm, n=1, where (a) and (c) represent the longitudinal oscillation with wave vector  $k_{x\circ}\approx 1.92$  nm and  $k_{x\circ}\approx 5.77$  nm (c) and (d) represent the transverse oscillation with wave vector  $k_{x\circ}\approx 1.92$  nm and  $k_{x\circ}\approx 5.77$  nm, for values of polarisation parameters  $\alpha=1,\beta=0$ , for different values of the Gaussian bandwidth d=0.1,0.13,0.17,0.26 nm.



**Figure 5.** Position operator as a function of time for a single layer of graphene nanoribbon width D=0.52 nm, n=1, where (a) and (c) represent the longitudinal oscillation with wave vector  $k_{x\circ}\approx 1.92$  nm and  $k_{x\circ}\approx 5.77$  nm (c) and (d) represent the transverse oscillation with wave vector  $k_{x\circ}\approx 1.92$  nm and  $k_{x\circ}\approx 5.77$  nm, for values of polarisation parameters  $\alpha=1$ ,  $\beta=1$ , for different values of the Gaussian bandwidth d=0.1,0.13,0.17,0.26 nm.

As a result of setting the pseudo-polarization values to  $\alpha = 1$  and  $\beta = 1$ , it is possible to deduce that the quantum state of the initial motion of electrons in the two sublattices A and B is simultaneous. This implies that the probability of electron presence is the same in both sublattices. This is seen in Figure 6, where it is clear that there is no fluctuation of the Average expected value in either direction, indicating that the ZBW phenomenon is not realized at these levels. This is obvious in panels a and b of the figure. While the electrons are in their initial motion, there is no constructive interference between the wave and the negative energy values. As a consequence, there is a linear connection between the position values and the time. An increase in the starting wave vector  $k_{x^{\circ}}$  causes this linearity to become more evident, as seen in Figure 5 (c, d). As was mentioned before, this does not have a direct impact on the oscillation, which decreases as time t continues, suggesting that motion is still occurring.

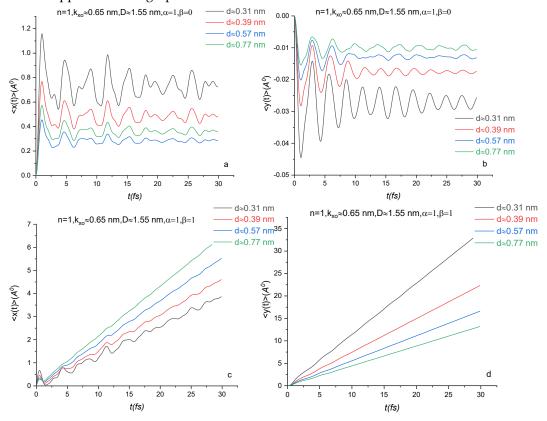
When the width of the graphene nanoribbon is increased to D = 1.04 nm, as shown in figure 6, we detect a consistent and steady oscillation behavior that is comparable to the one shown in fig.4. The starting wave vector  $k_{x_0}$  does not seem to have any noticeable influence; nevertheless, the width of the nanoribbon led to a drop in the maximum oscillation amplitude, which went from  $1.4A^{\circ}$  in to  $1.2A^{\circ}$  in. Figure 7 displays the data that demonstrates the irregularity of the oscillation period at the beginning of the movement.



**Figure 6.** Position operator as a function of time for a single layer of graphene nanoribbon width D=1.04 nm, n=1, where (a) and (c) represent the longitudinal oscillation with wave vector  $k_{x^{\circ}}\approx 2.88$  nm, (c) and (d) represent the transverse oscillation with wave vector  $k_{x^{\circ}}\approx 2.88$  nm, for values of polarisation parameters  $\alpha=1$ ,  $\beta=0$ , for different values of the Gaussian bandwidth d=0.21,0.26,0.35,0.52 nm.

In the case of an armchair nanoribbon with a width of D=0.52 nm, where  $\alpha=1$  and  $\beta=0$ , the oscillatory behaviour consistently occurs in both the longitudinal and transverse orientations. The figures c and d in Figure 5 demonstrate that linear oscillation is readily apparent when the values of  $\alpha$  and  $\beta$  are equal to one. This phenomenon takes place in a transverse orientation that is directly proportional to the width of the wave packet, while in the longitudinal direction, it is inversely proportional. In Figure 7, we can see that an armchair graphene nanoribbon with D=1.55 nm has oscillatory behaviour. Figures. 5(a and b) demonstrate that when the parameters  $\alpha=1$  and  $\beta=0$ , the longitudinal oscillation seems to be relatively unequal. On the other hand, the transversal oscillation is

transitory and has a modest amplitude. Figure 5(c, d) demonstrates that the conductive armchair graphene nanoribbon with D=0.52 nm showed linear oscillation at  $\alpha=\beta=1$ . This is apparent in the graph.



**Figure 7.** Position operator as a function of time for a single layer of graphene nanoribbon width D=1.55 nm, n=1, where (a) and (c) represent the longitudinal oscillation with wave vector  $k_{x\circ}\approx 0.65$  nm, for values of polarisation parameters  $\alpha=1,\beta=0$  (c) and (d) represent the transverse oscillation with wave vector  $k_{x\circ}\approx 0.65$  nm, for values of polarisation parameters  $\alpha=1,\beta=1$ , for different values of the Gaussian bandwidth d=0.31,0.39,0.57,0.77 nm.

#### 4. Conclusion

This study presents a comprehensive theoretical analysis of the Zitterbewegung (ZBW) phenomenon in armchair graphene nanoribbons, employing the Heisenberg representation within a long-wavelength approximation framework. The dynamic behavior of Dirac electrons was examined under varying physical parameters, including nanoribbon width, Gaussian wave packet width, pseudo-spin polarization, and initial wave vector. The findings reveal that ZBW manifests as transient, intrinsic oscillations with a characteristic lifetime of approximately 30 femtoseconds. These oscillations exhibit strong dependence on the structural and electronic parameters of the system: increasing ribbon width or wave packet spread reduces amplitude. The study highlights the significant influence of pseudo-spin configuration on the realization of the ZBW effect. Overall, these results contribute to a deeper understanding of relativistic quantum behavior in low-dimensional materials and offer promising insights for the development of ultrafast graphene-based quantum and nanoelectronic devices.

#### Declaration of competing interest

The authors declare that they have no competing interests.

### CRediT authorship contribution statement

Bashar. H. Azeez: Investigation, Software, Data curation, Writing - Original Draft.

Research data

Not applicable.

Supplementary material

Not applicable.

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Availability of data and materials

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