Zitterbewegung near new Dirac points in graphene superlattices

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Abstract

New Dirac points may appear when periodic potentials are applied to graphene, and there are many interesting effects near them. Here we investigate the Zitterbewegung effect of fermions described by a Gaussian wave packet in graphene superlattice near these points. The Zitterbewegung near different Dirac points has similar characteristics, while fermions near new ones have different group velocities in both $x$- and $y$-direction, which causes the different properties of the Zitterbewegung near them. We also investigate the Zitterbewegung effect influenced by multi Dirac points, and get the evolution with changing potential. Our results suggest that graphene superlattice may provide an appropriate system to study the Zitterbewegung effect near new Dirac points experimentally.

Keywords: Zitterbewegung, Dirac points, graphene superlattice

(Some figures may appear in colour only in the online journal)

Introduction

Zitterbewegung (ZB), put forward by Schrödinger [1], is a theoretical prediction of relativistic quantum mechanics, which is a high frequency trembling motion of an electron in vacuum and resulted from the interference between the positive and negative energy states. It is still difficult to directly observe ZB of the electron in free space through experiments due to its extreme high frequency.

Interestingly, the concept of ZB can also be applied in some non-relativistic system, because of the similarity between the relativistic electron and two interacting bands in a solid [2, 3]. ZB phenomenon has been predicted theoretically in variety of systems, such as semiconductors [4], superconductors [5], carbon nanotubes [6, 7], topological insulators [8], some optical systems [9–11], ultracold atoms [12], Weyl semimetals [13], MoS$_2$ [14], graphene [8, 15–22], as well as the spin–orbit coupling material [8, 23]. Shi et al. provided a general method to derive the analytical expression for the ZB effect then use it to investigate ZB in many different systems [8].

There is also an experimental observation of ZB using Bose–Einstein condensate [24]. Although it is difficult to observe ZB of electron in graphene because of its high frequency and low amplitude, the ZB phenomenon may be observed under current experiment conditions when a 1D periodic potential applies to it [18]. For this reason, it is significant to investigate ZB in 1D periodic graphene superlattices.

In this paper, we investigate the ZB phenomenon near new Dirac points of fermions in graphene superlattices. By applying a periodic potential to monolayer graphene, its band structure will change, and in some specific conditions, new Dirac points will appear [25–30]. Few works has been focused on ZB near these new Dirac points. When a periodic potential applies to graphene, the group velocity of the fermions turns to be highly anisotropic, and it has been illustrated that the $y$-direction group velocity will decrease but $x$-direction remain unchanged near original Dirac point. Nevertheless, near new Dirac points, both $x$- and $y$-direction group velocities will decrease [27–29], and then influence ZB effect remarkably.

In the following, we concentrate on the different features of ZB when fermions are near different Dirac points and described by a Gaussian wave packet, which are influenced by group velocities, wave packets and distance between the fermion and Dirac points. It is demonstrated that ZB has similar features and change rules near different Dirac points, but original Dirac point is special because of the symmetry...
and unchanged x-direction group velocity. The decrease of group velocities in two directions will affect ZB remarkably. These influences depend on the directions of oscillations in real space and initial momenta of wave packets. The evolution of ZB with changing initial momentum of fermions will be more complicated when there are new Dirac points. By investigating the ZB controlled by different Dirac points, we find that these oscillations may have the most prominent one when the Dirac points are far away, or be similar when the Dirac points are close, which can be regarded as controlled by all Dirac points. In addition, we study the evolution of ZB when the amplitude of periodic potentials and the number of Dirac points change. It indicates that the condition for obtaining ZB controlled by all Dirac points is to choose appropriate potential and wave packet and make all Dirac points inside it. Therefore, the ZB oscillation is controlled by the nearest Dirac point mainly in most instances and graphene superlattices may provide an appropriate system to research ZB near new Dirac point experimentally.

Model and method

We consider the low-energy electronic states of graphene, the Hamiltonian can be written as [31]

\[
H = h v_f (k_x \sigma_x + k_y \sigma_y), \tag{1}
\]

where \(v_f\) is Fermi velocity \(10^6\) m s\(^{-1}\), \(\sigma_x\) and \(\sigma_y\) are Pauli matrices and \(k\) is the wave vector from \(K\) point. For monolayer graphene, the position operator can be calculated by substituting equation (1) into \(x(t) = e^{i \vec{p} \cdot \vec{x}(0)} e^{-i \vec{p} \cdot \vec{t}}\) and its (1,1) component is

\[
x_{11}(t) = x_{11}(0) + \frac{k_x v_f^2}{2 \omega^2}[1 - \cos(2\omega t)], \tag{2}
\]

\[
y_{11}(t) = y_{11}(0) - \frac{k_y v_f^2}{2 \omega^2}[1 - \cos(2\omega t)], \tag{3}
\]

where \(\omega = \sqrt{(v_f k_x)^2 + (v_f k_y)^2}\). These equations can also be obtained by using general formula established by [8]. It has also been illustrated that ZB is controlled by effective Fermi velocity and the distance between fermion and Dirac point in previous research [9, 13, 16, 18].

We further consider a one-dimensional periodic potential along the x direction \(V(x) = V_0 \cos G_0 x\), which is applied to graphene, with the periodicity is \(L\) and \(G_0 = 2\pi / L\). The total Hamiltonian can read

\[
H = h v_f (k_x \sigma_x + k_y \sigma_y) + V(x) I, \tag{4}
\]

where \(I\) is a 2 \times 2 unit matrix. We take the form of \(V_0\) as \(V_0 = n \pi \frac{h v_f}{L}\). With different \(n\), the number of Dirac points in band structure is different, since new Dirac points appear in some \(V_0\). When \(n\) is a root of equation \(J_0(\frac{2 V_0}{n \pi v_f}) = 0\), where \(J_0\) is 0th Bessel function of the first kind, a pair of new Dirac points will appear in band structure [27]. Figure 1 shows band structures in different \(n\). We can see that the number of Dirac points is different in figure 1, and new Dirac points are symmetric about the original Dirac point. We mark the Dirac points from the original point of the coordinate system with 0, 1, 2...for convenience. These symbols are also marked in figure 1. Recent research have stated that graphene superlattice can be stable and provided various methods to fabricate superlattices [32]. Controllable new Dirac points could be generated by creating a lateral superlattice with tunable barriers in graphene by combination of two gates [33]. Periodic ripples on graphene surface could also induce potentials [34] and they are realized in experiments by thermal strain engineering [35, 36]. Therefore, it is possible to obtain stable potentials and new Dirac points in graphene, and then use them to investigate ZB experimentally.

One of the most important influences of periodic potential is that it can decrease the group velocities of electrons in real space, which can influence ZB oscillation. When a periodic potential is applied to monolayer graphene, the y-direction group velocity of fermions near original Dirac point decreases remarkably, but its x-direction group velocity does not change. Meanwhile, near new Dirac points, fermion’s x- and y-direction group velocities both decrease [27, 29]. We use \(f_x\) and \(f_y\) to indicate the change of group velocities, and \(v_x = f_x v_f\), \(v_y = f_y v_f\). They can be obtained by calculating the slope of band structure in momentum space [29]. In particularly, for cosine potential, \(f_y = J_0(\frac{2 V_0}{n \pi v_f})\) when fermion is near original Dirac point in first Brillouin zone [28].

We use the same method and substitute equation (4) into \(x(t) = e^{i \vec{p} \cdot \vec{x}(0)} e^{-i \vec{p} \cdot \vec{t}}\) to get (1,1) component of position operator. They will have the same form as equations (2) and (3), but different effective Fermi velocity and location of Dirac points when periodic potential applies to graphene. We rewrite them to make periodic potential’s influences clearer.

\[
x_{11}(t) = x_{11}(0) + \frac{f_x k_x v_f^2}{2 \omega^2}[1 - \cos(2\omega t)], \tag{5}
\]

\[
y_{11}(t) = y_{11}(0) - \frac{f_y k_y v_f^2}{2 \omega^2}[1 - \cos(2\omega t)], \tag{6}
\]

where \(\omega = \sqrt{(f_x v_f k_x)^2 + (f_y v_f k_y)^2}\), \(k_x = k_x - k_Dx\), \(k_y = k_y - k_Dy\). Here \((k_Dx, k_Dy)\) is the location of Dirac point in momentum space, and \(k_x\) and \(k_y\) are the components of the wave vector from Dirac point. Note that \(k_x\) and \(k_y\) are different from \(k_x\) and \(k_y\) respectively because new Dirac points are not at original point anymore. \(f_x, f_y\) indicate the changes in the x- and y-direction effective Fermi velocities respectively, with \(v_x = f_x v_f\), \(v_y = f_y v_f\). We can find that the motion of the fermion consists of an oscillation with frequency \(2\omega\).

We consider ZB near \(K'\) point starting from Hamiltonian when wave vector is close to \(K'\) point [37]:

\[
H = h v_f (k_x \sigma_x - k_y \sigma_y) + V(x) I. \tag{7}
\]

The group velocities also change near \(K'\) point like \(K\) point under potential. Using the same method as the \(K\) point we can get

\[
x_{11}(t) = x_{11}(0) - \frac{f_x k_x v_f^2}{2 \omega^2}[1 - \cos(2\omega t)], \tag{8}
\]

and it has the same expression as the equation (5) but just in the opposite direction. It is reasonable because the band
structures near $K$ and $K'$ points are the same, and the group velocities near them both change because of potential. However, for a given electron, since it has different wave vector from $K$ or $K'$ point, its displacement near these points may be different. In the following, we only study ZB near $K$ point due to the similarity and the large distance between these points.

We assume that the initial state of Dirac fermions can be described by a Gaussian wave packet [38, 39]

$$
\psi(\vec{r}, 0) = \frac{d}{2\pi^{3/2}} \int d^2k_0 e^{-\frac{i}{\hbar}d^2(k_x-k_0)^2 - \frac{d^2}{\hbar^2}(k_y-k_0)^2} e^{i\vec{k}_0 \cdot \vec{r}} (1) \text{, (9)}
$$

where $d$ is the width of the packet, and $(k_0, k_0)$ is the center of the packet in momentum space. For simplicity, if we do not indicate $k_0$, it will be 0. The unit vector $(1,0)$ is a convenient tool, and it can be created experimentally in quantum simulation experiments [40]. The real packets obtained in solids are even non-Gaussian such as a combination of few Hermite functions [41] and irregular function [7]. The center and width of Gaussian wave packet may influence ZB remarkably, since the center represents the initial location of an electron and the width represents the spread range of wave packet. Therefore, other non-Gaussian wave packets are perhaps also considered. However, Gaussian wave packets are the simplest cases. We should take an appropriate width of wave packet to research each Dirac point’s influences on ZB or ZB controlled by all Dirac points commonly. Firstly, we take a large $d$ to make wave packet’s width not too large in momentum space to avoid ZB being influenced by all Dirac points commonly. Then we take an appropriate $d$ to ensure that all Dirac points can be inside a wave packet in momentum space, so we can find laws of ZB controlled by all Dirac points.

The group velocities of fermions need to be considered. Near original Dirac point, we take $v_x = v_y$ and $v_x = f_x v_t = |J_0(\frac{2\kappa_x}{\hbar\nu_{\text{in}}})| v_t$ [28], and these velocities are not changed along with the motion of fermions since that band structure is linear about $k_x$ near original Dirac point. Near 1st new Dirac points, we do not have a equation to calculate $f_x$ and $f_y$, and they will change along with the motion of fermion, since band structure is not linear anymore. We get them by calculating the $k_x$- and $k_y$-direction slope at the location of wave packet’s center in band structure as $f_x$ and $f_y$ respectively.

Figure 1. Band structures of (a) graphene and (b)-(d) graphene superlattices with different $V_0$, where $V_0 = n \pi \frac{\hbar v}{L}$ with $n = 2$ (b), 4 (c), 6 (d) respectively. Energy is in units of $\epsilon_0 = \frac{\hbar v}{2a}$ and $k_0$ is in units of $a^{-1}$. Here $a$ is lattice constant of graphene and $L = 100a$. It demonstrates that new Dirac points appear in specific potentials. All new Dirac points are symmetric about the original one.

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We also notice that both two directions’ group velocities will change when potentials are applied to graphene in two directions [26]. Our method can also be used for this situation and may obtain similar properties.

Although the cosine potential is only a convenient tool for calculation and is hard to create experimentally, δ potential is equivalent to cosine one in principle and can be realized by electric field between electrodes [42, 43]. One can investigate ZB with δ potential in experiment to represent cosine one.

Since the influences on ZB of potentials are originated by the change of fermions’ group velocities, one can get \( f_x \) and \( f_y \) to reflect these effects and research ZB once the band structure can be obtained even under more complicated potentials. For example, band structure of graphene superlattices under square potential may also have new Dirac points and their \( x \)- and \( y \)-direction group velocities also decrease near them [29, 30]. We can obtain \( f_x \) and \( f_y \) from band structures to investigate ZB.

**Results and discussion**

We first study ZB controlled by each Dirac point independently. We take \( V_0 = 4\pi \frac{\hbar}{T} \), which \( L = 100a \) and \( a \) is lattice constant of graphene. The band structure is shown in figure 1(c) and here \( L = 100a \). \( f_x \) and \( f_y \) are calculated in the way mentioned in model and \( d = 150a \).

![Figure 2](image-url)

**Figure 2.** The \( x \)- and \( y \)-direction ZB oscillations near original Dirac point (a), (c) and 1st new one (b), (d) with different \( k_{0x} \) or \( k_{0y} \) but the same distance from wave packet’s center to Dirac point when \( V_0 = 4\pi \frac{\hbar}{T} \). The band structure is shown in figure 1(c) and here \( L = 100a \). \( f_x \) and \( f_y \) are calculated in the way mentioned in model and \( d = 150a \).

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First, we assume the distance from the centers of wave packets to Dirac points in momentum space is the same, and then it is reasonable that ZB has similar properties near different points, which is shown in figures 2(a) and (b). In these two figures, the oscillations have similar shapes, but different period, amplitude and attenuation, because fermions near new Dirac points have different group velocities. We also find that with increasing \( k_{0y} \), the amplitude of oscillation initially increases then decreases, and the period always decreases near both original and new Dirac points. It is also demonstrated that decreasing \( k_{0y} \) leads to smaller attenuation. It is understandable that ZB oscillation is caused by the interference between positive and negative energy states, the smaller energy gap causes this interference much easier. In equations (10) and (11), it is seen that the frequency is nearly proportional to \( k_{0y} \), but the amplitude is nearly proportional to \( k_{0x} \) or \( k_{0y} \). For this reason, ZB cannot appear when wave packet is at Dirac point in momentum space.

It is also shown that the amplitude and period change more remarkably with increasing \( k_{0y} \) in figure 2(b), because near new Dirac point, group velocities change with \( k_{0y} \), but remain constant near the original one. Therefore, the oscillation will evolve according to the rule mentioned above with \( k_{0y} \) near the original Dirac point, but evolve more complicatedly near...
the 1st new one. It is influenced by \( k_{0y} \) and group velocities simultaneously.

Figures 2(c) and (d) show the \( y \)-direction oscillations with different \( k_{0x} \) and a fixed \( k_{0y} \). With increasing \( k_{0x} \), it is seen that the amplitude, period and attenuation of ZB have similar properties with \( x \)-direction oscillation. However, near the 1st new Dirac point, the \( y \)-direction ZB oscillation has larger amplitude and period. Thus, one can choose the \( y \)-direction oscillation with \( k_{x} \)-direction initial momentum to observe ZB near the new Dirac points more easily.

Besides the decay shown in figure 2, what is originated from the electron localization and also influenced by wave packets, decoherence processes can also cause an exponential decay controlled by decoherence time \([7]\). This effect has been studied using density matrix formalism recently \([44, 45]\) and decoherence time is on the level of 10 fs approximatively \([46]\). In our research, the periods of oscillations are of order \( 10^{1} \rightarrow 10^{3} \) fs and decided by group velocities, so the periods may be close to the decoherence time with some specific velocities. Thus, the decay from decoherence processes need to be considered in some cases, especially for velocity that makes period be close to decoherence time.

Previous works illustrated that \( f_{y} \) increases the amplitude and period of ZB when fermions are near the original Dirac point and move along \( k_{y} \)-direction initially in momentum space \([18]\). In our research, fermions’ \( x \)-direction group velocities also change, and initial momentum may be in \( k_{x} \)-direction. To understand effects of \( f_{x} \) and \( f_{y} \) more explicitly, we show ZB without \( f_{x} \) or without \( f_{y} \) when fermions are near new Dirac point in figures 3(a), (b), and set some specific \( f_{x} \) and \( f_{y} \) in figures 3(c) and (d). Figure 3(c) shows both \( f_{x} \) and \( f_{y} \) can increase the period but the influence of \( f_{x} \) is more remarkable when the initial momenta are along \( k_{x} \)-direction. Opposite conclusion can be obtained from figure 3(d). In figure 3(c), we can also find that the oscillations have larger amplitude for \( f_{x} \) but than that for \( f_{x} = 1 \), but the smaller one for \( f_{y} \). Figure 3(d) exhibits the opposite property. Because the energy gap depends on the \( x \)-direction group velocity mainly if wave packets move along \( k_{y} \)-direction in momentum space. This conclusion is also suitable for the \( y \)- and \( k_{y} \)-directions. The decrease of the band structure’s slope in one direction leads to a smaller gap along this direction, then it causes the stronger interference. Meanwhile, in equations (10) and (11), the frequency \( 2\omega' \) is nearly proportional to group velocity. However, when \( f_{x} \) and \( f_{y} \) exist simultaneously, the amplitude will be proportional to one of them and then decrease. These properties are main influences of the anisotropy in graphene superlattices.

Assume wave packets’ centers be symmetric about original or new Dirac points respectively in figures 4(a) and (b). Figure 4(a) shows the same oscillations at symmetric position, but the amplitude and period are different in figure 4(b). Notice that when \( k_{0y} = 0.057a^{-1} \) in figure 4(b), the oscillation has a large period due to the small slope of band structure. In this condition, the ZB oscillation is affected by the original Dirac point. Therefore, ZB can be controlled by both new and original Dirac points in some specific conditions.

We also take \( V_{0} = 2\pi \frac{n_{f}}{T} \) (without new Dirac points) and \( V_{0} = 4\pi \frac{n_{f}}{T} \) (with new Dirac points) to find the differences about ZB when there are new Dirac points or not. In figure 4(c), we can see that the oscillations evolve with \( k_{0y} \) as the rule shown in figure 2(a) due to unchanged group
Figure 4. The ZB oscillation when wave packets are symmetric about original Dirac point (a) and 1st right new one (b). (c) and (d) are oscillation when $V_0 = 2\pi \frac{\hbar v}{L}$ and $V_0 = 4\pi \frac{\hbar v}{L}$ respectively with the same $k_0$, $f_1 = 1$, $f_2 = 0.224$ in (c) and they are gotten by calculating slope of band structure in (d). Other parameters are the same as figure 2.

Figure 5. The ZB oscillation when $V_0 = 2.43\frac{\pi \hbar v}{L}$ (a) and $V_0 = 4\frac{\pi \hbar v}{L}$ (b). Here original, right and left indicate ZB controlled by original Dirac point, 1st right and left new Dirac points respectively. $d = 100a$, $k_0 = 0.001a^{-1}$ in (a) and $k_0 = 0.025a^{-1}$ in (b), $f_1 = 1$, $f_2 = 0.013$ in (a) and they are gotten by the way as figure 2 in (b). Other parameters are the same as figure 2. (c) and (d) Are ZB oscillations controlled by original Dirac point and all Dirac points respectively with different $V_0$ in units of $e_0 = \pi \frac{\hbar v}{L}$. $f_1 = 1$ and $f_2$ are obtained by calculating $J_0(\frac{V_0}{\hbar v G_0})$. Other parameters are the same as (a).
velocities. In figure 4(d), there are two similar oscillations at different $k_0y$ due to the presence of the new Dirac points. The oscillation evolution rules with $k_0y$ become complex.

Secondly, ZB oscillations may be controlled by multi Dirac points. It is known that there are three Dirac points when $V_0 = 2.405 - 5.52\pi \frac{\hbar \nu}{T}$ [27]. We take $V_0 = 2.39, 2.40, 2.41, 2.42, 2.43\pi \frac{\hbar \nu}{T}$, so that we can get the evolution of ZB with the number of Dirac points. To make all Dirac points inside wave packet, we take $d = 100a$ and $k_{0y} = 0.001a^{-1}$, then get $f_x = 1$ and $f_y = J_0\left(\frac{2V_0}{\hbar \nu G_0}\right)$. Since $k_{0y}$ and the slope are small, and slope change slowly, we regard $f_x$ and $f_y$ as constant in this sense.

We first compare ZB oscillation controlled by three Dirac points respectively when $V_0 = 2.43\pi \frac{\hbar \nu}{T}$ and $4\pi \frac{\hbar \nu}{T}$. In figure 5(a) we can see that all oscillations have similar period and amplitude when Dirac points are close to each other and all inside the wave packet, so we can superpose them to an oscillation. The oscillations have opposite directions because two new Dirac points are at different sides of wave packet. However, ZB oscillations in figure 5(b) have clear distinctions, since Dirac points are far away from each other and not all inside the wave packet. If we superpose these oscillations, it is equivalent to add a perturbation to the largest one. Thus, the oscillation is controlled by the nearest Dirac point mainly. We could also obtain that all points cannot be inside a wave packet, the ZB oscillation will be controlled by the nearest Dirac points mainly, and wave packet to obtain ZB controlled by multi Dirac points.

Conclusions

In summary, we have studied the ZB oscillation of fermions near new Dirac points in graphene superlattices. Compared with the ZB near the original Dirac point, ZB near new Dirac points can have some different properties due to different group velocities. Additionally, we can choose appropriate potential and wave packet to obtain ZB controlled by multi Dirac points. However, if Dirac points are so far away in momentum space that all points cannot be inside a wave packet, the ZB oscillation will be controlled by the nearest Dirac points mainly, and we have to choose a smaller width of wave packet to make all Dirac points inside it then cause low amplitude. We should adjust potential to make band structure have Dirac points which are not far away to obtain ZB influenced by all Dirac points.

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