Zitterbewegung in time-reversal Weyl semimetals

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Received 1 February 2018, revised 22 April 2018
Accepted for publication 3 May 2018
Published 21 May 2018

Abstract

We perform a systematic study of the Zitterbewegung effect of fermions, which are described by a Gaussian wave with broken spatial-inversion symmetry in a three-dimensional low-energy Weyl semimetal. Our results show that the motion of fermions near the Weyl points is characterized by rectilinear motion and Zitterbewegung oscillation. The ZB oscillation is affected by the width of the Gaussian wave packet, the position of the Weyl node, and the chirality and anisotropy of the fermions. By introducing a one-dimensional cosine potential, the new generated massless fermions have lower Fermi velocities, which results in a robust relativistic oscillation. Modulating the height and periodicity of periodic potential demonstrates that the ZB effect of fermions in the different Brillouin zones exhibits quasi-periodic behavior. These results may provide an appropriate system for probing the Zitterbewegung effect experimentally.

Keywords: Zitterbewegung, Weyl semimetals, time-reversal

(Some figures may appear in colour only in the online journal)
modes, i.e., linearly dispersive Weyl fermions that are robust and have no symmetry protection [26–29]. The linearly dispersive and gapless properties imply that there should be ZB oscillations in WSMs, and the topological characteristics suggest that these oscillations will be stable near the Weyl nodes.

Apart well as being a promising possible platform for the ZB effect, chiral fermions give rise to quantum anomalies that originate from the monopole nature of the Weyl nodes [30–32]. It is natural to investigate the dynamics of Weyl fermions with different chirality, and studies of this frontier problem with broken inversion symmetry in an optical lattice have demonstrated an unusual velocity in the semimetal and a steady ZB effect in the band insulator [33].

In this paper, we examine the trajectories of Weyl fermions with broken spatial-inversion symmetry in a low-energy system under a one-dimensional periodic potential. We find that the massless Weyl fermions are generated near the Brillouin zone boundary along the direction of the potential in reciprocal space. Their group velocities reduce to zero in the other two dimensions, and the magnitudes of the amplitude and period of the oscillations are on the nm- and ps-scale, respectively. This is sufficiently large to provide ZB oscillations that may be observed through radiated transverse electric field [34] emitted by the trembling motion of the electron. By using a Gaussian wave packet, we derive analytic results for the time dependence of the average displacement of Weyl fermions. Our results show that the evolution of fermions consists of rectilinear motion and ZB oscillations. By changing the parameter of the potential, we also demonstrate that they depend strongly on the effective velocity. Interestingly, the character of the Bessel function means that the maximum amplitude and period of the ZB effect exhibit a quasi-periodic behavior with the height $V_0$ and period $L$ of the potential, and the parameter of the potential ranges across the low-value region when the fermion is away from the center of the Brillouin zone. Moreover, the motion is sensitive to the chirality of the system and the relative displacement of the fermion and the Weyl node. As a result, the two nonequivalent Weyl nodes in time-reversal WSMs are too far apart to influence the ZB effect of the fermion simultaneously.

Model and method

Compared with a time-reversal broken WSM, nonmagnetic WSMs generated by breaking the spatial-inversion symmetry could be more easily investigated using angle-resolved photoemission spectroscopy (ARPES), because the magnetic domains need not aligned [35]. To date, the only means of discovering WSMs is to use ARPES to detect Fermi arcs in the surface [36, 37]. For low-energy Weyl fermions with broken inversion symmetry, the Hamiltonian for each node can be written as [38]

$$H_0 = \sum_{j=x,y,z} sh\nu_j(\kappa_j + sb_j)\sigma_j, s = \pm 1,$$

(1)

where $\nu_j$ are the Fermi velocities in three directions, $\kappa_j$ are the three components of the wave vectors, $\sigma_j$ are the Pauli matrices, and $s = \pm 1$ labels the chirality of each node. Clearly, the vector $\vec{b} = (b_x, b_y, b_z)$ quantifies the separation of the two nodes in the momentum space.

The ZB effect originates from the interference between the conduction and valence bands in solid materials. One can see a lower Fermi velocity could enhance the interference near the Dirac points or Weyl nodes. Previous studies [39, 40] have demonstrated that the periodic potential could decrease the Fermi velocity dramatically in graphene. The cosine potential have a substantive character of periodic potential, and in theoretical study, it should be easy to have some analytical solutions and address detailed problems if a cosine potential is considered. On the other hand, the effective cosine potential, in principle, is equivalent to the square or $\delta$ periodic potential in the experiment, which is produced via electric field between electrodes [8, 41]. Thus, let us assume a potential $V(x) = V_0\cos G_0x$ along the $x$-direction with periodicity $L$, where $G_0 = 2\pi/L$, is applied to the WSM. The Hamiltonian $H$ can be written as

$$H = \sum_{j=x,y,z} sh\nu_j(\kappa_j + sb_j)\sigma_j + IV(x),$$

(2)

where $I$ is the $2 \times 2$ identity matrix. It has been shown that massless Weyl fermions are generated near the Brillouin zone boundary $\vec{G}_m/2$ with $\vec{G}_m = mG_0\vec{x}$, and the group velocities reduce to zero in the $y$- and $z$-directions in the extreme case [39]. The low-energy Hamiltonian for fermions can be written as

$$\tilde{H}_m = \sum_{j=x,y,z} sh\nu_j(\kappa_j + sb_j)\sigma_j + I\hbar v_m G_0 m/2,$$

(3)

with $\vec{k} \equiv \vec{r} + \vec{G}_m/2$, $|\vec{k}| \ll G_0$ and $\vec{x} = (1, f_m, f_m)$, where $f_m = J_m(\frac{2\pi}{\hbar v_m G_0})$ is determined by the periodic potential $V(x)$ with $J_m$ as the $m$th Bessel function of the first kind [40]. The derivation of this expression is given in the appendix. The difference between the Hamiltonian in equation (1) and that in equation (3), apart from a constant energy term, is that the velocities of fermions moving along the $y$- and $z$-directions have changed from $\nu_y$, $\nu_z$ to $f_m\nu_y$, $f_m\nu_z$, respectively. This means that fermions near $\vec{G}_m/2$, different from the original massless Weyl fermions in equation (1), are massless particles with anisotropic velocities depending on the propagation direction.

Time-reversal WSMs have an even number of Weyl pairs, and the distance between two nonequivalent Weyl points is sufficiently far that they cannot influence the ZB effect of the fermion simultaneously. Thus, we consider only one Weyl point. The time-dependent position operator of fermions near the generated Weyl points in the Heisenberg picture $\vec{r}(t) = e^{i\omega t/\hbar}\vec{r}(0)e^{-i\omega t/\hbar}$ is a $2 \times 2$ matrix. Applying the Baker–Hausdorff lemma [42],...
\[ \vec{r}(t) = \vec{r}(0) + (\hbar i / h) \left[ \hat{H}_m, \vec{r}(0) \right] \]
\[ + \frac{(i \hbar / 2)^2}{m} \left[ \hat{H}_m, \left[ \hat{H}_m, \vec{r}(0) \right] \right] + \cdots \]
\[ = \sum_{n=0}^{\infty} \frac{(i \hbar / 2)^n}{n!} \left[ \hat{H}_m, \left[ \hat{H}_m, \cdots \left[ \hat{H}_m, \vec{r}(0) \right] \right] \right] , \tag{4} \]

and from equation (3), the commutator of the operators \( \hat{H}_m \) and \( \vec{r}(t) \) reads
\[ \left[ \hat{H}_m, \vec{r}(0) \right] = \sum_{j=x,y,z} sh\lambda_j \sigma_j \vec{e}_j \]
\[ = -ih \sum_{j=x,y,z} \lambda_j \gamma_j \sigma_j \vec{e}_j , \tag{5} \]

where \( i \) is the imaginary unit and \( \vec{e}_j \) are the three components of the unit vectors. We then obtain explicit results for the three coordinate components of \( \vec{r}(t) \):
\[ x_1(t) = x_1(0) + \frac{sf_{m} k_{1x} v_x}{\hbar^2} t + \frac{f_{m} k_{1x} v_x}{\hbar^2} \left[ 1 - \cos(2\omega t) \right] \]
\[ - \frac{sf_{m} k_{1x} v_x}{\hbar^2} \sin(2\omega t) , \tag{6} \]
\[ y_1(t) = y_1(0) + \frac{sf_{m} k_{1y} v_x}{\hbar^2} t - \frac{f_{m} k_{1y} v_x}{\hbar^2} \left[ 1 - \cos(2\omega t) \right] \]
\[ - \frac{sf_{m} k_{1y} v_x}{\hbar^2} \sin(2\omega t) , \tag{7} \]
\[ z_1(t) = z_1(0) + \frac{sf_{m} k_{1z} v_z}{\hbar^2} t + \frac{sf_{m} k_{1z} v_z}{\hbar^2} \left[ 1 - \cos(2\omega t) \right] \]
\[ - \frac{sf_{m} k_{1z} v_z}{\hbar^2} \sin(2\omega t) , \tag{8} \]

where the relative displacement between the fermion and the Weyl node is \( k'_{1j} = k_j + s_h b_{1j} = x, y, z \) and the effective frequency is \( \omega = \sqrt{(k'_{1x})^2 + (f_{m} k_{1y} v_x)^2 + (f_{m} k_{1z} v_z)^2} \). One can see that the motion of the fermion consists of a rectilinear component and an oscillation with frequency 2\( \omega \). Comparing equations (6)–(8), we find that the velocity in the y and z-directions is more sensitive to the factor \( f_{m} \) than that in the \( x \)-direction (see the second term of these equations), and the oscillation is influenced by the chirality of fermions (see the last term of these equations). Furthermore, the rectilinear motion is the classical velocity of the fermion.

The initial state of the fermion is described by a Gaussian wave packet [5, 43]
\[ \varphi(\vec{r}, 0) = \left( \alpha / 2 \pi \right)^{3/2} e^{-\frac{(\vec{r} - \vec{r}_0)^2}{4\alpha^2}} \int d^3k e^{i\vec{k}\cdot\vec{r}} \left( \begin{array}{c} 1 \\ 0 \end{array} \right) , \tag{9} \]

where \( \alpha \) denotes the width of the packet, and \( \vec{r}_0 \) is the center wave vector of the packet. The unit vector \((1, 0)\) is a convenient choice [43]; the average of the \((1, 1)\) component of \( \vec{r}_{11} \) is written as

\[ \hat{r}_{11}(t) = \langle \varphi(\vec{r}, 0) | \vec{r}(t) | \varphi(\vec{r}, 0) \rangle \]
\[ = \frac{\alpha^3}{\pi^{3/2}} \int \int \int \hat{r}_{11}(t) e^{-\frac{(\vec{k} - \vec{k}_0)^2}{4\alpha^2}} d\vec{k}_1 d\vec{k}_2 d\vec{k}_3 . \tag{10} \]

For simplicity, the packet is centered at \( \vec{k}_0 = (0, 0, 0) \) so that there is an appropriate momentum to generate observable ZB oscillations [44] when the nodes are away from the origin of the coordinates.

**Results and discussion**

TaAs is a natural WSM. It belongs to the nonsymmetric group \( I_4/mmd \) and has a body-centered-tetragonal structure, that lacks spatial-inversion symmetry. The three-dimensional trajectories of TaAs fermions under a cosine potential in the \( x \)-direction are plotted in figure 1 as \( \vec{b} = (1.735, 0.025, 0) \) \( \tilde{A}^{-1} \) [45], the packet is centered at \( \vec{k}_0 = (1.735, 0.055, 0.03) \). One can see that the fermions with different chiralities (green and red lines) have opposite directions of motion, and the different chirality introduces a different phase to the system, but the trajectory of the fermion in the anisotropic situation (blue...
line) changes drastically. The magnitudes of the amplitude and period of the oscillations are on the nm- and ps-scale, respectively. To understand these unusual traits, we first study the displacement of the right-handed \( (s = +1) \) fermion in the \( x \)-direction as a function of time for a Gaussian wave packet with a different width \( \alpha \) at \( \vec{b} = (0.03, 0.03, 0.03) \) Å\(^{-1}\), as shown in figure 2(a). In our preliminary calculation, the Fermi velocity was set to \( 1 \times 10^8 \) cm s\(^{-1}\) for the isotropic system. As shown in the figure, (i) there are nearly no oscillations when \( \alpha \) is small, (ii) the maximum amplitude of ZB oscillations and the velocity of the rectilinear motion in the \( x \)-direction increase with the width of the wave packet, whereas the period of the ZB oscillations are almost constant, and (iii) the oscillations have a transient character and may decay in several femtoseconds. These results show that the ZB behavior is a damped oscillation with the exponential decay factor in equation (10) and depends quite critically on the value of \( \alpha \), consistent with previous work [9, 46]. Thus, the packet width \( \alpha \) was set to 160 Å in the subsequent simulations.

Next, we focus on the relationship between the separation of two nodes and the motion of the fermion. The calculated displacements of the three coordinate components of the right-handed fermion are plotted as a function of time in figures 2(b)–(d), respectively. We can see that the rectilinear motion of the fermion vanishes when the node is in the \( x - y \) plane \( (b_z = 0) \). This is consistent with the behavior of 2D materials [9] in which the \( \sigma_z \) term is absent. The time terms of equations (6)–(8) suggest that the time term is zero when \( k'_z = k_z + b_z \approx b_z = 0 \). Therefore, we conclude that the rectilinear motion originates from the additional momentum determined by the position of the Weyl node in the \( z \)-direction. In addition, the amplitude and period of the ZB effect depend sensitively on the relative displacement of the fermion and the Weyl points \( k'_j \); in other words, the smaller the value of \( b_j \) the smaller the energy gap, leading to a lower ZB frequency and a stronger oscillating amplitude.

From figure 1, one can also find that fermions with different chiralities have opposite direction of motion. To further understand this behavior, figures 3(a) and (b) plot the displacement of fermions with different chiralities for the three coordinate components under the same parameters. As discussed above, the velocities of the rectilinear motion are equal and opposite since the time terms of equations (6)–(8) have the chirality factor \( s \). The amplitude and period of the ZB oscillations are the same for the different chiralities in all components, whereas the phase difference between the left-handed \( (s = -1) \) and the right-handed \( (s = +1) \) fermions is \( \pi \) because of the opposite sign. This suggests that the chirality strongly changes both the direction of the rectilinear motion and the phase of the oscillation.
Figure 3. Average displacement of (a), (c), (d) a right-handed, and (b) a left-handed fermion in three coordinate components at $\alpha = 160^\circ A$ and $\vec{b} = (0.03, 0.03, 0.03) \text{ Å}^{-1}$; (a) and (b) are from the isotropic system, (c) is from the anisotropic system, and (d) is the same as (c) but with a periodic potential with $f_1 = 0.1$.

Figure 4. Evolution of right-handed fermions in the anisotropic system with periodic potentials across several $f_1$ values in (a) $x$-direction, (b) $y$-direction, and (c) $z$-direction. (d) Maximum amplitude and period of the ZB oscillations in the $x$-direction as a function of $f_1$; the Weyl points were positioned at $\vec{b} = (0, 0.03, 0.03) \text{ Å}^{-1}$. 

effective velocity $v_{\text{eff}} = \sqrt{v_x^2 + v_y^2 + v_z^2}$, which depends on the anisotropy. In addition, the change in velocity of the rectilinear motion in the $y$- and $z$-directions is more drastic than that in the $x$-direction, which is consistent with the time terms in equations (6)–(8).

We now study the right-handed fermion in the anisotropic system with the periodic potential in the case of $m = 1$ (see figure 3(d)). Comparing figures 3(c) and (d), one can see that the amplitude and period of oscillations are slightly larger than that of the system without the periodic potential, which is due to the large value of $v_x$. Therefore, we calculate the average displacement of the right-handed fermion as a function of time at $\vec{b} = (0, 0.03, 0.03)$ Å$^{-1}$ across several $f_1$ values, as shown in figures 4(a)–(c). As $f_1$ decreases, the period and amplitude of the ZB oscillations increase in the $x$-direction, and the attenuation of the oscillations becomes slower. However, there is no change in the $y$- and $z$-directions, because the amplitude of oscillations is only inversely proportional to $f_m$ in the $x$-direction (consider equations (6)–(8) with $k'_x = k_x + b_x = 0$). In contrast, there is a positive correlation between the velocities of the rectilinear motion and $f_1$ in the $y$- and $z$-direction, but this vanishes in the $x$-direction. From equations (6)–(8), it is apparent that the time term is zero in the $x$-direction, but proportional to $f_m$ in the $y$- and $z$-directions.

The long-range electron–electron interaction causes a ‘logarithmic’ correction to the Fermi velocity in WSMs [47, 48]. Thus, the ZB effect will show ‘logarithmic’ dependence on the frequency in accordance with equations (6)–(8). Similarly, the periodic potential strongly affects the ZB effect by changing the Fermi velocity. We further investigate the maximum amplitude and period of the ZB oscillations as a function of $f_1$ in the $x$-direction (see figure 4(d)). The maximum amplitude of the oscillations decreases from approximately 143 to 78 Å, and the period decreases from approximately 2.5 ps to 45 fs, as $f_1$ changes from 0.01 to 0.5. To understand the relationship between the ZB effect and the periodic potential directly, figure 5 shows the period and maximum amplitude of the ZB oscillations in the $x$-direction with different values of the cosine potential parameters $V_0$ and $L$ in the different Brillouin zones. The change in the effective velocity causes the period and the maximum amplitude of the ZB oscillations to vary.
quasi-periodically with the height $V_0$ or periodicity $L$, and their maxima decrease and become a constant with increasing height $V_0$ or periodicity $L$. Furthermore, the period changes more drastically than the maximum amplitude because of the overlap of the trigonometric and exponential functions. From figure 5, one can see that the ranges of $V_0$ and $L$ become broad in the low-value region, and the peaks of the period and maximum amplitude are equal when the fermion is away from the center of the Brillouin zone. All these fascinating behaviors derive from the character of the Bessel function, and our results may provide an appropriate and stable system for probing the ZB effect experimentally.

**Summary**

We have studied the rectilinear motion and ZB oscillation of fermions with broken spatial-inversion symmetry in a low-energy WSM. Compared with the situation in 2D materials such as graphene, the rectilinear movement has a unique character in a 3D WSM because of the additional momentum in the $z$-direction, which allows us to identify the chiral fermion via its direction. Furthermore, the smaller separation of the Weyl nodes results in a lower ZB frequency and a stronger oscillating amplitude, and the different chiralities of fermions in WSMs gives rise to a π phase in the ZB oscillations. Additionally, the effective velocity can be diminished by modulating the periodicity or height of the cosine potential in the $x$-direction when the momentum is zero in the same direction. This gives rise to a steady ZB effect that may pave the way to investigating its behavior under perturbations.

**Acknowledgments**

TH and TM were supported in part by NSCFs (grant nos. 11774033 and 11334012) and the Fundamental Research Funds for the Center Universities, grant no. 2014KJJC826. We also acknowledge computational support from the HSSC of Beijing Normal University. L-GW was supported by Zhejiang ProvincialNatural Science Foundation of China under Grant No. LD18A040001, and the grant by National Key Research and Development Program of China (No. 2017YFA0304202); it was also supported by the National Natural Science Foundation of China (grants No. 11674284 and U1330203), and the Fundamental Research Funds for the Center Universities (No. 2017FZA3005).

**Appendix**

This appendix presents a derivation of equation (3) in the anisotropic case, using the unitary matrix

$$U_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\alpha(x)/2} & -e^{i\alpha(x)/2} \\ e^{-i\alpha(x)/2} & e^{i\alpha(x)/2} \end{pmatrix}, \quad \text{(A.1)}$$

where $\alpha(x)$ is written as

$$\alpha(x) = 2 \int_0^x V(x')dx'/\hbar v_0, \quad \text{(A.2)}$$

with the period potential $V(x')$, the reduced Planck constant $\hbar$ and the Fermi velocity $v_0$. From equation (2), the Hamiltonian $H' = U_1^\dagger H U_1$ reads

$$H' = \hbar v_0 \left( e^{i\alpha(x)} \left( -\partial_x + i\partial_y \right) \right). \quad \text{(A.3)}$$

By applying the two pseudospin states near the Brillouin zone boundary ($\vec{r} \pm \vec{G}_m/2$) as basis functions, we obtain the unitary matrix

$$U_2 = \begin{pmatrix} e^{i(\vec{r}+\vec{G}_m/2)^2} & 0 \\ 0 & e^{i(\vec{r}−\vec{G}_m/2)^2} \end{pmatrix}. \quad \text{(A.4)}$$

After a similarity transformation $H'' = U_2^\dagger H' U_2$, the Hamiltonian $H$ is further given by

$$H'' = \hbar v_0 \left( -\partial_x + mG_0/2 \right) \left( -\partial_x + i\partial_y \right) \beta \left( -\partial_x + i\partial_y \right), \quad \text{(A.5)}$$

where we use $-i\partial_y = k_y \gg \kappa_y$ ($j = x, y, z$), and $\beta = e^{-imG_0x+i\alpha(x)}$. Using the Fourier expansion

$$e^{i\alpha(x)} = \sum_{m=-\infty}^{\infty} f_m(V)e^{imG_0x}, \quad \text{(A.6)}$$

where $f_m(V)$ is determined by the period potential, the matrix $M_m$ derived from the Hamiltonian $H''$ can be written as

$$M_m = \hbar v_0 \left( f_m(\partial_x + i\partial_y) \right) \left( -\partial_x + i\partial_y \right), \quad \text{(A.7)}$$

Finally, employing a unitary transformation $M'_m = U_3^\dagger M_m U_3$ with the unitary matrix

$$U_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \quad \text{(A.8)}$$

the result is

$$M'_m = \hbar v_0 \left( k_x \sigma_x + f_m k_y \sigma_y + f_m k_z \sigma_z \right) + i\hbar v_0 mG_0/2. \quad \text{(A.9)}$$

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