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Electronic Bloch oscillation in a pristine monolayer graphene

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ABSTRACT

In a pristine monolayer graphene subjected to a constant electric field along the layer, the Bloch oscillation of an electron is studied in a simple and efficient way. By using the electronic dispersion relation, the formula of a semi-classical velocity is derived analytically, and then many aspects of Bloch oscillation, such as its frequency, amplitude, as well as the direction of the oscillation, are investigated. It is interesting to find that the electric field affects the component of motion, which is non-collinear with electric field, and leads the particle to be accelerated or oscillated in another component.

In the solid state physics, Bloch oscillation is an important phenomenon. It is usually involved with the coherent motion of quantum particles in periodic structures. For example, an electron (a matter wave) suffers this effect in a periodic lattice subjected to a constant external field. This phenomenon is predicted from quantum mechanics in very early days [1,2] and has been demonstrated in various fields of physics, such as semiconductor superlattices [3,4], photonic crystals [5], cold-atom systems [6], and acoustic waves [7]. However, electric domains lead to the instability of the electric field and destroy the Bloch oscillation in the semiconductor superlattices, which requires a complex design to suppress electric domains [8].

On the other hand, since its discovery in 2004, graphene has attracted a tremendous amount of interest due to its unique properties that may promise a broad range of potential applications [9–14]. Recently, many theoretical and experimental investigations focus on the graphene-based superlattices with electrostatic potentials or magnetic barriers [15–23], including periodic [24–27], aperiodic [28–30], disorder [31], and sheet arrays system [32]. Different from the common semiconductors, graphene superlattices can maintain a stable electric field due to the uniform population of the quantum well, which is induced by the back gate voltage, and some researchers have investigated the electronic Bloch oscillations in a structure with periodic potentials [33], a graphene nanoribbon with a hybrid superlattice [34], graphene superlattices with multiple Zener tunneling [35], a tilted honeycomb lattice for the localized Wannier-Stark states [36], as well as the Bloch oscillations in the gapped graphene. It has been demonstrated that Bloch oscillations in graphene are different from that in common semiconductors, since the electron in graphene is described by Dirac rather than the Schrödinger equation. Moreover, the Bloch oscillation in graphene superlattices has potential applications on such as infrared detectors and lasers. One important issue still remains, that is, what does the electronic Bloch oscillation behavior in the gapless graphene?

Many aspects of Bloch oscillation can be obtained by a single band description via using the dispersion relation to derive the semi-classical velocity of the particle. In this work, based on the electronic structure under tight-binding approximation, we derive the motion of an electron in pristine monolayer graphene subjected to a constant external field. Within such a simple and efficient way, our results show several interesting phenomena of the electronic Bloch oscillation in graphene. For example, when the electric field is applied in one direction, the oscillation disappears in the x direction in a special condition, while it never happens in the y direction. Due to the linear dispersion relation, the amplitude and period of the oscillation are doubled as the particle passes through Dirac points, and its trajectory is almost a circle. In the following, we firstly derive the general formula of the motion of an electron based on the dispersion relations, and then we analyze the properties of the Bloch oscillation.

A monolayer graphene is well known for its honeycomb structure, and its dispersion relation can be written as [11]

$$\mathcal{E}(k) = \pm\varepsilon\sqrt{3 + f(k)}, \tag{1}$$

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where $f(k) = 2\cos(\sqrt{3}ak_y) + 4\cos(\frac{\sqrt{3}}{2}ak_y)\cos(\frac{3}{2}ak_x)$. $a \approx 1.42$ Å is the carbon-carbon distance, and $\varepsilon \approx 2.5$eV is related to Fermi velocity ($v_F \approx 10^6$ m/s), $\hbar v_F = \frac{3}{2}\varepsilon a$ [11]. The signs "+" and "−" are, respectively, corresponding to the electron and hole energy band, which touch together at Dirac points (DPs). From Eq. (1), it is easy to find that the DPs are located at $[\frac{4n\pi}{3a}, \frac{2}{\sqrt{3}a}(2n \pm \frac{2}{3})\pi]$, $[\frac{2}{3a}(2n+1)\pi, \frac{2}{\sqrt{3}a}(2n \pm \frac{1}{3})\pi]$ with $n = 0, \pm1, \pm2, \cdots$. According to $v = \frac{1}{\hbar}\frac{\partial\mathcal{E}(k)}{\partial k}$ [37], we can readily have $v = (v_x, v_y)$ as the function of k_x and k_y,

$$v_x = \frac{\mp 3\varepsilon a \sin(\frac{3}{2}ak_x)\cos(\frac{\sqrt{3}}{2}ak_y)}{\hbar\sqrt{3 + f(k)}},$$
$$v_y = \frac{\mp\sqrt{3}\varepsilon a[\sin(\sqrt{3}ak_y) + \sin(\frac{\sqrt{3}}{2}ak_y)\cos(\frac{3}{2}ak_x)]}{\hbar\sqrt{3 + f(k)}}, \quad (2)$$

which show that v_x and v_y are the periodic functions of k_x and k_y, and the sign "−" ("+") is corresponding to the velocities of electron (hole or hole-like electron). Basically, the Berry curvature should affect the trajectory of a wave packet undergoing Bloch oscillations in optical lattice [38], while in present system, the anomalous contribution does not show up since the Berry curvature is just a monopole like contribution at the Dirac point for gapless graphene [39]. When a constant electric field $E = (E_x, E_y)$ is applied along the layer of graphene, Dóra et al. showed that the velocity of massless Dirac electrons was pinned to the Fermi velocity in a finite field, and the electric field moved the Dirac point around in momentum space. Those special features imply that Dirac electrons in the electric field could be treated as critical particles, and their motion is a drift transport, so they move ballistically and leave their footprints [40]. Thus, the semiclassical approach should be valid, and we employ the electronic motion equation $\hbar\frac{dk(t)}{dt} = -eE$ to describe the motion of Dirac electron, which survives as

$$k_x(t) = k_x(0) - \frac{eE_x}{\hbar}t, \quad k_y(t) = k_y(0) - \frac{eE_y}{\hbar}t, \quad (3)$$

where $k_x(0)$ and $k_y(0)$ are the initial wave-vector values. Substituting Eq. (3) into Eq. (2), we can obtain the dynamic formula for v. Therefore using Eqs. (2)–(3), we can analyze the motion of the electron or hole in graphene under the constant electric field. In particular, from Eq. (1), one can see that tight-binding approximations could describe both the conduction band and valence band, and the Dirac point moves continuously in momentum space and have not been destroyed under an electric field. On the other hand, previous study has also found that the behavior of the electron obtained by tight-binding is consistent with that from Bloch equations as the electron passes the Dirac point [41,42]. Thus, our formula is valid for dynamics involving band-crossing points. Since the direction of the electric field E can be chosen arbitrarily, we shall firstly discuss the electronic motion when E is only along the x (*case I*) or y (*case II*) direction and then generalize it to an arbitrary direction (*case III*).

Case I: E along the x direction. In this case $E_y = 0$, so we have $k_y(t) = k_y =$ constant, and $k_x(t) = k_x(0) - \frac{eE_x}{\hbar}t$. Assuming $k_x(0) = 0$, the dynamic formula of v_x and v_y are

$$v_x(t) = \frac{\mp 3\varepsilon a \sin(-\frac{2\pi}{T}t)\cos(\frac{\sqrt{3}}{2}ak_y)}{\hbar G(t)}, \quad (4a)$$

$$v_y(t) = \frac{\mp\sqrt{3}\varepsilon a[\sin(\sqrt{3}ak_y) + \sin(\frac{\sqrt{3}}{2}ak_y)\cos(-\frac{2\pi}{T}t)]}{\hbar G(t)}, \quad (4b)$$

where $G(t)=\sqrt{3 + 2\cos(\sqrt{3}ak_y) + 4\cos(-\frac{2\pi}{T}t)\cos(\frac{\sqrt{3}}{2}ak_y)}$, and $T = \frac{4\pi}{3}\frac{\hbar}{|aeE_x|}$. From Eqs. (4a)–(4b), it is easy to see that $v(t+T) = v(t)$ with T being the period of the motion. The frequency and circular frequency of the Bloch oscillation are generally given by

$$\nu_B = \frac{1}{T} = \frac{3}{4\pi}\frac{|aeE_x|}{\hbar} \text{ and } \omega_B = 2\pi\nu_B = \frac{3}{2}\frac{|aeE_x|}{\hbar}, \quad (5)$$

respectively. According to the expression of v, the time-dependent position $r(t)$ of the electron is $r(t) = r(0) + \int_0^t v dt$, and here we assume the initial position $r(0) = 0$, i.e., $x(0) = 0$ and $y(0) = 0$. After a simple derivation, we obtain $x(t) = C - \frac{s}{eE_x}G(t)$ where C is an integration constant satisfying $x(0) = 0$. For $y(t)$, we have to numerically calculate the following

$$y(t) = -\frac{2\sqrt{3}\varepsilon\omega_B}{3eE_x} \times \int_0^t \frac{\sin(\sqrt{3}ak_y) + \sin(\frac{\sqrt{3}}{2}ak_y)\cos(-\omega_B t)}{G(t)}dt. \quad (6)$$

According to the formula of $x(t)$, we can have

$$x_{\max} = C - \frac{\varepsilon}{|eE_x|}\sqrt{3 + 2\cos(\sqrt{3}ak_y) - 4|\cos(\frac{\sqrt{3}}{2}ak_y)|},$$
$$x_{\min} = C - \frac{\varepsilon}{|eE_x|}\sqrt{3 + 2\cos(\sqrt{3}ak_y) + 4|\cos(\frac{\sqrt{3}}{2}ak_y)|}. \quad (7)$$

Therefore, the amplitude of the oscillation along x direction, $L_x = |x_{\max} - x_{\min}|$, is given by

$$L_x = \frac{\varepsilon}{|eE_x|}||1 + 2\cos(\frac{\sqrt{3}}{2}ak_y)| - |1 - 2\cos(\frac{\sqrt{3}}{2}ak_y)||. \quad (8)$$

When $|\cos(\frac{\sqrt{3}}{2}k_y a)| \geq \frac{1}{2}$, L_x has its maximum value: $L_x^{\max} = \frac{2\varepsilon}{|eE_x|}$. When $\frac{\sqrt{3}}{2}ak_y = (n + \frac{1}{2})\pi$, $L_x^{\min} = 0$. According to Eq. (8), if $E_x = 4.61$ mV/nm, (we set $\varepsilon = 2.5$ eV in the whole paper), $L_x^{\max} \approx 1084$ nm with $\nu_B \approx 237$ GHz. The amplitude and period of the clean graphene is larger than those of superlattices based on the graphene with the gapped band structure, which are around 30 nm and 0.8 ps, respectively [35].

Fig. 1(a) and (b) demonstrate the time dependence of v_x and v_y with different values of k_y. It is found that when $\frac{\sqrt{3}}{2}ak_y = \frac{\pi}{3}$, shown as the dash red lines, the electron passes through the DPs, and the period of v_x and v_y is doubled. Because the electron passes through the DPs, the electron transits into another band and behaves as a hole-like electron. After a period in another band, the hole-like electron behaves as the electron again. Therefore, the period of the velocity becomes twice time, and correspondingly the amplitude is also doubled. This is quite different from the gapped case, where the Bloch oscillations originate from the interference between the electron and hole states [35]. There is an interesting phenomenon that, the oscillation along the x direction disappears although E is still along the x direction when $\frac{\sqrt{3}}{2}ak_y = (n + \frac{1}{2})\pi$. Meanwhile, since $v_y \neq 0$, the oscillation in the y direction remains, see the solid blue lines ($\frac{\sqrt{3}}{2}ak_y = \frac{\pi}{2}$) in Fig. 1(a) and (b). In other hands, if $\frac{\sqrt{3}}{2}ak_y = n\pi$, we have $v_y = 0$. It means that the oscillation in y-axis disappears and the oscillation in x-axis remains, see the solid dark lines in Fig. 1(a) and (b).

The corresponding electron's trajectories are shown in Fig. 1(c), where we demonstrate the trajectory of an electron within three periods on the graphene layer. It is clear that, when the electron (or hole) passes through the DPs, its amplitude is doubled

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