Electronic Bloch oscillation in a pristine monolayer graphene

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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 dynamic formula of semi-classical velocity is derived analytically, and then many aspects of conventional Bloch oscillation, such as the frequency, amplitude, as well as the direction of the oscillation, are investigated. It is interesting to find that the electric field should affect the component of motion which is non-collinear with electric field, making the particle accelerated or oscillated in another component.

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\textsuperscript{[1–3,5–12]}. Recently, many theoretical and experimental investigations focus on the graphene-based superlattices with electrostatic potentials or magnetic barriers\textsuperscript{[6–11]}, including periodic\textsuperscript{[12–15]}, aperiodic\textsuperscript{[16–18]}, and disorder system\textsuperscript{[19]}. Some researchers have also investigated the electronic Bloch oscillations in a structure with periodic potentials\textsuperscript{[20]} and a graphene nanoribbon in presence of a periodic mass potential\textsuperscript{[21]}.

One important issue still remains opening is that, what does the electronic Bloch oscillation behave in the pristine graphene without any potential structures or nanoribbons?

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\textsuperscript{[22–25]} and has been demonstrated in various fields of physics, such as semiconductor superlattices\textsuperscript{[24, 25]}, photonic crystals\textsuperscript{[27]}, cold-atom systems\textsuperscript{[28]}, and acoustic waves\textsuperscript{[29]}. Different from the common semiconductors, the electron in graphene are described by Dirac rather than the Schrödinger equation, and then its Bloch oscillation naturally is an interesting issue to be investigated.

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 paper, 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. 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\textsuperscript{[3]}

\[ \mathcal{E}(k) = \pm \sqrt{3} + f(k), \]  

where \( f(k) = 2 \cos(\sqrt{3}ak_y) + 4 \cos(\frac{\sqrt{3}}{2}ak_y) \cos(\frac{4}{3}ak_x). \) \( a \approx 1.42\AA \) is the carbon-carbon distance, and \( \varepsilon \approx 2.5 \text{eV} \) is related to Fermi velocity \( (v_F \approx 10^6 \text{m/s}) \), \( h \gamma_F = \frac{1}{2} \varepsilon a \textsuperscript{[3]} \). 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 \( \{ \frac{4n\pi}{3n+1}, \frac{2n\pi}{2n+1} \} \), \( \{ \frac{2n\pi}{2n+1}, \frac{2n\pi}{2n+1} \} \) with \( n = 0, \pm 1, \pm 2, \ldots \). According to \( v = \frac{\hbar \mathcal{E}(k)}{m} \), we can readily have \( v = (v_x, v_y) \) as the function of \( k_x \) and \( k_y \),

\[ v_x = \mp 3\varepsilon a \left[ \sin\left(\frac{\sqrt{3}}{2}ak_y\right) \cos\left(\frac{4}{3}ak_x\right) \right] \frac{\hbar}{\sqrt{3} + f(k)}, \]

\[ v_y = \mp 3\varepsilon a \left[ \sin\left(\sqrt{3}ak_y\right) + \sin\left(\frac{4}{3}ak_y\right) \cos\left(\frac{4}{3}ak_x\right) \right] \frac{\hbar}{\sqrt{3} + f(k)}, \]  

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).

When a constant electric field \( E = (E_x, E_y) \) is applied along the layer of graphene, the electronic motion equation \( \frac{dk(t)}{dt} = -eE \) survives as

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

where \( k_x(0) \) and \( k_y(0) \) are the initial wave-vector values. Substituting Eq. 1 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. 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 $k_y(t) = k_y = \text{constant}$, and $k_x(t) = k_x(0) - \frac{e}{\hbar} E_y t$. Assuming $k_x(0) = 0$, the dynamic formula of $v_x$ and $v_y$ are

$$v_x(t) = \pm 3 \varepsilon a \sin(-\frac{2\pi}{3} t) \cos\left(\frac{\sqrt{3}}{2} a k_y\right) \frac{hG(t)}{\hbar}$$

$$v_y(t) = \pm \sqrt{3} \varepsilon a [\sin(3a k_y) + \sin(\frac{\sqrt{3}}{2} a k_y) \cos(-\frac{2\pi}{3} t)] \frac{hG(t)}{\hbar}$$

where $G(t) = \sqrt{3 + 2 \cos(\sqrt{3} a k_y) + 3 \cos(-\frac{2\pi}{3} t) \cos(\frac{\sqrt{3}}{2} a k_y)}$, and $T = \frac{4\pi}{3 \varepsilon a E_x}$. From Eq. 4, 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

$$\nu_B = \frac{1}{T} = \frac{3}{4\pi} \frac{|a e E_x|}{\hbar}$$

$$\omega_B = 2\pi \nu_B = \frac{3}{2} \frac{|a e E_x|}{\hbar}$$

respectively. According to the expression of $v$, the time-dependent position $r(t)$ of the electron is $r(t) = r(0) + \int_0^t v(t) dt$, 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 $x(t) = C - \frac{\varepsilon}{|e E_x|} G(t)$ where $C$ is an integration constant satisfying $x(0) = 0$. For $y(t)$, we have to numerically calculate the following

$$y(t) = -\frac{2\sqrt{3} \varepsilon \nu_B}{3 e E_x} \times \int_0^t \frac{\sin(\sqrt{3} a k_y) + \sin(\frac{\sqrt{3}}{2} a k_y) \cos(-\omega_B t)}{G(t)} dt$$

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

$$x_{\max} = C - \frac{\varepsilon}{|e E_x|} \sqrt{3 + 2 \cos(\sqrt{3} a k_y) - 4 |\cos(\frac{\sqrt{3}}{2} a k_y)|}$$

$$x_{\min} = C - \frac{\varepsilon}{|e E_x|} \sqrt{3 + 2 \cos(\sqrt{3} a k_y) + 4 |\cos(\frac{\sqrt{3}}{2} a k_y)|}$$

(7)

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

$$L_x = \frac{\varepsilon}{|e E_x|} |1 + 2 \cos(\frac{\sqrt{3}}{2} a k_y)| - |1 - 2 \cos(\frac{\sqrt{3}}{2} a k_y)||.$$ (8)

When $|\cos(\frac{\sqrt{3}}{2} a k_y)| \geq \frac{1}{2}$, $L_x$ has its maximum value, $L_x^{\max} = \frac{2\varepsilon}{|e E_x|}$; and when $\frac{\sqrt{3}}{2} a k_y = (n + \frac{1}{2})\pi$, $L_x^{\min} = 0$. According to Eq. 8 if $E_x = 4.61 \text{ mV/mm}$ [21], (we set

$\varepsilon = 2.5 \text{ eV in the whole paper }$, $L_x^{\max}$ $\approx 1084 \text{ nm with } \nu_B \approx 376 \text{ GHz}$.)

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 $\frac{\sqrt{3}}{2} a k_y = \frac{\pi}{4}$, shown as the dash red lines, the electron shall pass through the DPs, and the period of $v_x$ and $v_y$ shall be doubled. Because the electron passes through the DPs, the electron should transit into another band and behave as a hole-like electron. After a period in another band, the hole-like electron shall behave as the electron again. Therefore the period of the velocity becomes twice time, and correspondingly the amplitude shall be doubled. There is an interesting phenomenon that, the oscillation along the $x$ direction disappears although $E$ is still along the $x$ direction when $\frac{\sqrt{3}}{2} a k_y = (n + \frac{1}{2})\pi$. Meanwhile, since $v_y \neq 0$, the oscillation in the $y$ direction remains, see the solid blue lines ($\frac{\sqrt{3}}{2} a k_y = \frac{\pi}{3}$) in Fig. 1(a) and (b). In other hands, if $\frac{\sqrt{3}}{2} a k_y = n\pi$, we shall 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 shall be doubled and its trajectory is approximately a circle, see the dash red lines ($\frac{\sqrt{3}}{2} a k_y = \frac{\pi}{5}$) in Fig. 1(c). In general, the motion in the $x$ and $y$ directions may oscillate, but its trajectory

\begin{center}
\begin{figure}
\includegraphics[width=\textwidth]{fig1.png}
\caption{(Color online) The time dependence of $v_x$ (a), $v_y$ (b) and (c) the trajectories of the electron (or hole-like electron) on the graphene sheet for different $k_y$ at $\frac{\sqrt{3}}{2} a k_y = 0$ (solid dark line line ), $\frac{\sqrt{3}}{2} a k_y = \frac{\pi}{4}$ (dash-dot-dot magenta line), $\frac{\sqrt{3}}{2} a k_y = \frac{\pi}{4}$ (dash red line), $\frac{\sqrt{3}}{2} a k_y = \frac{\pi}{3}$ (dot green line), and $\frac{\sqrt{3}}{2} a k_y = \frac{\pi}{3}$ (solid blue line). The electric field $E$ is along the $x$ direction.}
\end{figure}
\end{center}
is very complex and depends on the initial value of $k_x$. For example, its trajectory should be a helix (see short dash green line for $\sqrt{2}/3 ak_y = \frac{5}{12}\pi$); or go further and further with variational velocity, its trajectory should be like a sine function (see dash-dot-dot magenta line for $\sqrt{2}/3 ak_y = \frac{3}{4}$).

Case II: $E$ along the $y$ direction. In this case, $E_x = 0$, so we have $k_x(t) = k_x = \text{constant}$ and $k_y(t) = k_y(0) - \frac{eE}{\hbar}t$. Assuming $k_y(0) = 0$, the dynamic formula read as

$$v_x(t) = \mp 3e\sin\left(\frac{3}{2}k_x\right)\cos\left(-\frac{\pi}{3}\right)\hbar G'(t),$$

$$v_y(t) = \frac{\mp \sqrt{3}e\sin\left(-\frac{4\pi}{3}t\right) + \sin\left(-2\pi t\right)\cos\left(\frac{3}{2}k_x\right)}{\hbar G'(t)}$$

(9)

where $G'(t) = \sqrt{3 + 2\cos(-\frac{4\pi}{3}t) + 4\cos\left(\frac{3}{2}k_x\right)\cos(-\frac{2\pi}{3}t)}$ and the period of the motion $T' = \frac{4\pi}{|k_x| E_x}$. From Eq. 9 we still have $v(t + T') = v(t)$. The frequency and circular frequency of Bloch oscillation are accordingly

$$\nu'_B = \frac{1}{T'} = \frac{\sqrt{3}}{4\pi} \frac{|eE|}{\hbar}$$

and $\omega'_B = \frac{\sqrt{3}}{2} \frac{|eE|}{\hbar}.$

(10)

From Eqs. 5 and 9, we can see that the direction of the electric field shall affect the frequency of Bloch oscillation. Similar to Case I, $y(t) = C' - \frac{eE}{\hbar} G'(t)$, where $C'$ is an integration constant satisfying $y(0) = 0$. For $x(t)$ we have to numerically calculate

$$x(t) = \frac{2\sqrt{3}e\omega'_B}{eE_y} \int_0^t \sin\left(\frac{3}{2}k_x\right)\cos\left(-\omega'_B t\right) G'(t) dt$$

(11)

The amplitude of the oscillation along the $y$ direction, $L_y = |y_{max} - y_{min}|$, is given by

$$L_y = \frac{e}{|eE_y|} \sqrt{5 + |4 \cos\left(\frac{3}{2}k_x\right)| - \left| 1 - \cos^2\left(\frac{3}{2}k_x\right) \right|},$$

(12)

which show that $L_y$ has its maximum value $L_{y_{max}} = \frac{3}{|eE_y|}$ when $\cos\left(\frac{3}{2}k_x\right) = \pm 1$, and $L_{y_{min}} = \frac{\sqrt{5}}{|eE_y|}$ when $\cos\left(\frac{3}{2}k_x\right) = 0$. If $E_y = 4.61$ mV/nm, then $L_{y_{max}} \approx 1627$ nm, $L_{y_{min}} \approx 671$ nm with $\nu_B \approx 137$ GHz.

Fig. 2(a) and (b) show the Lissajous figures of $v_x$ and $v_y$ with different values of $k_x$. When $\sqrt{2}/3 ak_x = 0$, the electron shall pass through the DPs and shall behave as a hole-like electron, and after a period of time it shall behave as an electron again, and its amplitude is increased accordingly. At this case when $-\omega't \in \left[2n + \frac{\pi}{2}, 2n + \frac{3\pi}{2}\right]$, the particle behaves as a hole-like electron, otherwise it behaves as an electron.

Different from the case I, the oscillation along the $y$ direction never disappears when electric field is along the $y$ direction, and its amplitude never becomes zero. There is a special case that when $k_x = 0$, we find that $v_x = 0$. At this case the oscillation in the $x$-direction shall disappear. The corresponding trajectories within three periods are shown in Fig. 2(c) and (d).

Case III: $E$ along the arbitrary direction. At this case, the dynamics of the electron becomes much more complicated, since both $E_x$ and $E_y$ are not 0. Meanwhile, the dynamic properties of $v_x(t)$ and $v_y(t)$ are also related with the initial phase $k_x(0)$ and $k_y(0)$ and the ratio $E_x/E_y$.

$v_x$ and $v_y$ depend on the two periodic functions $\cos\left(\frac{3}{2}ak_x(0) - \frac{eE_y}{h}t\right)$ and $\cos\left(\frac{3}{2}ak_y(0) - \frac{eE_x}{h}t\right)$. Let $T_x$ denote the period of the former, and $T_y$ denote the period of the latter, so we have $T_x = \frac{4\pi}{3|eE_x|}$ and $T_y = \frac{4\pi}{3|eE_y|}$. If the ratio $T_x/T_y$ is rational, i.e. $T_x/T_y = \frac{m}{n}$, ($n$ and $m$ are integers), then $v_x(t)$ and $v_y(t)$ are periodic with the periods being $mT_y$ or $nT_x$. But if $T_x/T_y$ is irrational, $v_x(t)$ and $v_y(t)$ should not be periodic anymore: they should not have a finite period. In this case the motion is not a periodic oscillation, even though the particle may move back and forth.

Finally, we discuss the dynamics of electrons under the condition of $k_x(0) = k_y(0) = 0$ with some specific directions, where $x(0) = y(0) = 0$, $\alpha = \arctan(E_y/E_x)$, $E = |E|$, and $\omega_x = 2\pi/T_x$. The time dependence of $v_x$ and $v_y$ with different values of $\alpha$ are illustrated in Fig. 3(a) and (b), and the corresponding trajectories within $3T_x$ are shown in Fig. 3 (c). Due to the rotational symmetrical structure of graphene, it is easy to find that, when $\alpha = \frac{\pi}{6}$ (solid dark line) the direction of the electric field is equivalent to the $y$ direction, and the electron
shall also pass through DPs in this case; when $\alpha = \frac{3\pi}{4}$ (solid red line) the direction of the electric field is equivalent to the $x$ direction. When $\sqrt{\frac{7}{2}} a k_y = \frac{\pi}{4}$ (dash blue line), it is a general case, in which the electron is only moving within a single energy band.

In summary, we have derived the general formulas for the velocity of the electron in graphene subject to a constant electric field, and analyzed the dynamic properties of electron for some particular and interesting cases. When electric field is along $x$-axis and $y$-axis, we find Bloch oscillation in direction of electric field, and we address formulas for its amplitude and frequency. We also find that the electric field affect the motion in other direction, making the electron oscillating or moving forward with fluctuation in other direction. Moreover, the velocity is periodic in all directions in these two cases. Finally, we analyze the period of the motion and give the numerical result if electric field has an arbitrary direction. Our result should be a positive insight for experimentally observing the Bloch oscillation in a pristine graphene, which may facilitate the development of graphene-based electronics.

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