Double-periodic quasi-periodic graphene superlattice: non-Bragg band gap and electronic transport

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Abstract

Electronic band gap and transport in quasi-periodic graphene superlattice (GSL) of double-periodic sequence are investigated. It is found that such quasi-periodic structure can possess a zero-averaged wave-number (zero-\( \bar{k} \)) gap which is associated with an unusual Dirac point. Different from Bragg gap, the zero-\( \bar{k} \) gap is less sensitive to the incidence angle, and robust against the lattice constants. The locations of Dirac point and multi-Dirac-points in the GSLs of various sequences are also compared. The control of electron transport over the zero-\( \bar{k} \) band gap in GSLs may facilitate the development of many graphene-based electronics.

1. Introduction

Since the discovery of graphene in 2004, electronic band gap and transport in graphene have attracted considerable attention because of the intriguing physics as well applications in graphene-based nanoelectronics [1–4]. Graphene has a unique band structure with the conductance and valance bands touching at Dirac point, which leads to many unusual properties of transport [4], like half-integer quantum Hall effect, Klein tunnelling, and the minimal conductance. So far, the transport properties including Klein tunnelling and resonant tunnelling have been extensively investigated in various graphene-based heterostructures ranging from single barrier [5, 6] to superlattice with electrostatic potential and magnetic barriers [7–20].

Several works have been devoted to zero-averaged wave-number (zero-\( \bar{k} \)) gap, associated with the new Dirac point, in the band structure of graphene superlattices (GSLs) [8, 9, 15, 19, 20], since such unusual zero-\( \bar{k} \) gap is of benefit to the controllability of electronic transport. Different from Bragg gaps, the zero-\( \bar{k} \) gap emerged with new Dirac point is robust against the lattice constant, structural disorder [15], and external magnetic field [16]. In essence, the so-called zero-\( \bar{k} \) gap is analogous to the well-known zero-\( \bar{n} \) gap in the photonic crystal with positive and negative index materials [21], which results from zero (volume) averaged refractive index. Moreover, the structure ordering of quasi-periodic GSL is between periodic and disordered systems, which could give rise to many interesting and significant phenomena, for example, shrinkage of spectrum [22], fractal spectrum and self-similar behaviour [23–25]. In the 1990s, Domínguez-Adame et al [23] studied the electronic transport, electron localization length, and transmission spectrum in Fibonacci (FB) superlattice of narrow-gap III–V semiconductor. Recently, we have focused on the zero-\( \bar{k} \) gap and electronic transport in FB quasi-periodic GSL [19]. Briefly afterwards, Ma et al [20] found that the zero-\( \bar{k} \) gap also exists in other quasi-periodic GSL of the Thue–Morse (TM) sequence.

As we know, the main examples of quasi-periodic models include the FB, TM and double-periodic (DP) structures [26, 27]. These quasi-periodic superlattices can be generated by the following substitution rules: \( A \rightarrow AB \) and \( B \rightarrow A \) for FB, \( A \rightarrow AB \) and \( B \rightarrow BA \) for TM, and \( A \rightarrow AB \) and \( B \rightarrow AA \) for DP, where \( A \) and \( B \) are two different barriers in the quasi-periodic superlattice. The DP quasi-periodic superlattice is obviously different from FB and TM ones. But the number of barrier layers in the DP sequence increases as \( N = 2^n \) (like the TM sequence), where \( n \) indicates the iteration order, and barriers B appear always isolated (like the FB sequence) [27]. The electronic properties of FB, TM and DP lattice are of significance [28]. So it is worthwhile to study the electronic band gap and transport in DP GSL and make comparisons with different quasi-periodic systems. Combining the results in FB and TM GSL [19, 20], the controllable conductance and shot
noise in DP GSL may result in the practical applications of
electron transport in quasi-periodic GSL.

2. Theoretical model

Consider a graphene-based DP quasi-periodic superlattice
which is arranged by DP substitution rule, \( A \rightarrow AB \) and
\( B \rightarrow AA \), where \( A \) and \( B \) are two different barriers,
the parameters are denoted by the potential barrier height \( V_A \) and
width \( d_A \), the potential well height \( V_B \) and width \( d_B \). For an \( n \)-th
DP sequence, \( S_n \), it contains elements \( A \) and \( B \), and follows
the relation, \( S_n = S_{n-1}S_{n-1}^{-1} \) (for \( n > 1 \)) with
\( S_1 = AB \) and \( S_1^{-1} = AA \), which leads to \( S_2 = ABAA, S_3 =
ABABAAABAB, S_4 = ABABABAABAAABAB \) and so on.
The Hamiltonian of charge carriers near the \( K \) point inside a
monolayer graphene is given by, \( \hat{H} = -i\hbar \nabla \cdot \sigma \cdot \nabla + V(x) \),
where the Fermi velocity \( v_F \approx 10^6 \text{ m s}^{-1} \), and \( \sigma = (\sigma_x, \sigma_y) \)
are the Pauli matrices and \( V(x) \) denotes the potential barrier or
well. The solution of \( \hat{H} \), acting on the electronic pseudospin
wave functions, results in the transfer matrix [15]:

\[
M_j(\Delta x, E, k_y) = \begin{pmatrix}
\frac{\cos(q_j \Delta x - \theta_j)}{\cos \theta_j} & i \frac{\sin(q_j \Delta x)}{\cos \theta_j} \\
\frac{\sin(q_j \Delta x)}{\cos \theta_j} & \frac{\cos(q_j \Delta x + \theta_j)}{\cos \theta_j}
\end{pmatrix},
\]

which connects the wave functions at \( x \) and \( x + \Delta x \) inside
the \( j \)-th potential with \( \theta_j = \arcsin(k_y/k_j) \), where \( k_j =
(E - V_j)/\hbar v_F, k_j \), and \( q_j \) are the \( y \) and \( x \) components of
wavevector, \( q_j = \text{sign}(k_j)(k_j^2 - k^2)^{1/2} \) for \( k_j^2 > k^2 \),
otherwise \( q_j = i(k_j^2 - k^2)^{1/2} \). Noting that when the incident
energy satisfies \( V_B < E < V_A, \theta_A < 0, q_A < 0, \theta_B > 0 \) and \( q_B > 0 \)
for the propagating mode. Consequently, the transmission
coefficient \( t = t(E, k_y) \) is found to be

\[
t = \frac{2 \cos \theta_0}{(m_{22} e^{-\theta_0} + m_{11} e^{\theta_0}) - m_{12} e^{\theta_0} - m_{21}},
\]

where \( \theta_0 \) and \( \theta_i \) are incidence and exit angles, and \( m_{ij}(i, j =
1, 2) \) is the matrix element of total transfer matrix, \( X[S_n] =
\prod_{j=1}^{N} M_j(d_j, E, k_y) \). Introducing \( x_n = \text{Tr}[X[S_n]] \), we can
derive the iteration relation for the trace map of the \( n \)-th DP
sequence as follows [26]:

\[
x_{n+1} = x_{n-1}(x_n x_{n-1} - x_{n-2}^2 - 2) - x_n.
\]

In general, we can derive \( \cos(\theta, \Lambda_n) = x_n/2 \) from Bloch’s
theorem, where \( \Lambda_n = N_A d_A + N_B d_B \), \( N_A \) and \( N_B \) are
the numbers of barrier \( A \) and well \( B \) for an \( n \)-th DP sequence
as a unit cell. Once the transmission coefficient is obtained,
we can calculate the total conductance \( G \) [29] and the Fano
factor \( F \) [30] in terms of \( G = G_0 \int_{-\pi/2}^{\pi/2} T \cos \theta_0 \, d\theta_0, \)
and \( F = \int_{-\pi/2}^{\pi/2} T(1 - T) \cos \theta_0 \, d\theta_0 / \int_{-\pi/2}^{\pi/2} T \cos \theta_0 \, d\theta_0 \),
where \( T = |t|^2 \) and \( G_0 = 2e^2/\hbar v_F L_y/\hbar^2 \), with \( L_y \) the
width of the graphene stripe in the \( y \) direction.

3. Results and discussion

In figures 1(a) and (b), we plot the trace maps for quasi-
periodic GSL of DP sequences, \( S_n \), where parameters are \( (a) \)
\( d_A = d_B = 20 \text{ nm}, (b) d_A = 2d_B = 30 \text{ nm} \), the incidence
angle \( \theta_B = 20^\circ \), \( V_A = 50 \text{ meV}, V_B = 0 \text{ meV} \) and \( m = 12 \).
The grey-code bar in figure 1 gives different transmission
probabilities of these graphene-based structures, in which the
white regions present \( T = 0 \), whereas the dark regions present
\( T = 1 \). Similar to the results for FB and TM sequences
[19, 20], we find that there are several broad forbidden gaps
opening for each DP level, and the passing bands are split into
more and more subbands as the DP sequence order \( n \) increases.
Among these forbidden gaps, the centre position of the zero-\( k \)
gaps, which are denoted by a dashed red line, are almost the
same for different DP sequences in figures 1(a) and (b). These
zero-\( k \) gaps are different from Bragg gaps, because the position
and size of these gaps become stabilized with increasing DP
level number, see figure 1, and thus such gaps are robust against
the lattice parameters.
Figure 2. Electronic and structures for DP quasi-periodic GSL, \((ABAA)^{12}\), where \((a)\) \(d_A = d_B = 20\) nm, \((b)\) \(d_A = 2d_B = 30\) nm, and the other parameters are the same as those in figure 1. The horizontal dashed red line denotes the new Dirac point’s location.

Figure 3. Transmission spectra for DP quasi-periodic GSL, \((ABAA)^{12}\), where \((a)\) \(d_A/d_B = 1, d_A = 15\) nm (dashed black line), \(d_A = 20\) nm (solid red line), \((b)\) \(d_A/d_B = 2, d_A = 20\) nm (dashed black line), \(d_A = 30\) nm (solid red line), and the other parameters are the same as those in figure 1.

To understand aforementioned zero-\(\bar{k}\) gap better, we further calculate the electronic dispersion, for example the second DP sequence \((S_2 = ABAA)\), at any incidence angle

\[
\cos(\beta_x, \Lambda_2) = \frac{1}{2} \text{Tr}(M_A M_B M_A M_A),
\]

\[
= \cos(3q_A d_A) \cos(q_B d_B) + \frac{\sin \theta_A \sin \theta_B - 1}{\cos \theta_A \cos \theta_B} \times \sin(3q_A d_A) \sin(q_B d_B),
\]

where \(\beta_x\) is the \(x\) component of Bloch wave vector, and \(\Lambda_2 = 3d_A + d_B\) is the length of the unit cell. If \(3q_A d_A = -q_B d_B\), equation (4) becomes

\[
\cos(\beta_x, \Lambda_2) = 1 + \frac{1 - \cos(\theta_A - \theta_B)}{\cos \theta_A \cos \theta_B} \sin^2(3q_A d_A),
\]

which indicates that, when \(3q_A d_A = -q_B d_B \neq m\pi\) \((m = 0, 1, 2 \ldots)\) and \(\theta_A \neq 0\) (also \(\theta_B \neq 0\)), \(\cos(\beta_x, \Lambda_2) > 1\), so there is no real solution for \(\beta_x\), that is, existing band gap. At normal incident case \(\theta_A = \theta_B = 0\), this band gap will be closed, and two bands are touched at Dirac point. Figures 2\((a)\) and \((b)\) show the electronic band structures, where \((a)\) \(d_A = d_B = 20\) nm, \((b)\) \(d_A = 2d_B = 30\) nm, the white regions represent the forbidden gap, i.e. \(\cos(\beta_x, \Lambda_2) > 1\), while the passing bands are shown in the blue regions in which \(\cos(\beta_x, \Lambda_2) < 1\) is true. In figure 2 we demonstrate that a band gap opens exactly at energy \(E = 37.5\) meV (for \(d_A = d_B = 20\) nm) and \(E = 42.857\) meV (for \(d_A = 2d_B = 30\) nm) at oblique incidence, (i.e. \(k_y \neq 0\)), when the condition \(3q_A d_A = -q_B d_B \neq m\pi\) is satisfied. In the case of normal incidence (\(\theta_A = \theta_B = 0\)) the upper and lower bands linearly touch together, which forms a new double-cone Dirac point. In general, the location of new Dirac point in this case is determined by

\[
\bar{k} = \sum_{j=1}^{N} k_j d_j / \sum_{j=1}^{N} d_j = 0,
\]

\(3\).
which is valid for both periodic and aperiodic GSLs [9, 15, 19, 20]. That is the reason that we call an opened gap (also see figure 3), associated with the new new Dirac point, as the zero-averaged wave-number (zero-\(\bar{k}\)) gap. Based on equation (6), we achieve the new Dirac point located at

\[
E_n = \frac{V_A + V_B \cdot d_B/(\tau_n d_A)}{1 + d_B/(\tau_n d_A)},
\]

which depends on the ratio of numbers of layer A and B, that is, \(\tau_n = N_A/N_B\). Here we would like to emphasize that the location of Dirac point is generally dependent of the order \(n\). But when the TM sequence is considered, the location of Dirac point does not depend on the order \(n\) because of \(\tau_n = 1\) [20]. The different behaviours will be compared later in the different GSLs of FB, TM and DP sequences. Moreover, we see the Dirac point also depends on the ratio \(d_A/d_B\). As shown in figures 2(a) and (b), the position of Dirac point is shifted from \(E = 37.5\) meV for \(d_A/d_B = 1\) to \(E = 42.875\) meV for \(d_A/d_B = 2\). Furthermore, figure 3 shows the transmission spectra for DP quasi-periodic GSL, \((ABAA)^\infty\). It is demonstrated that the zero-\(\bar{k}\) gap is robust against the ratio of lattice parameters, \(d_A/d_B\), while other Bragg gaps are sensitive to lattice parameters. From the point of view of application, this provides the flexibility to control the electron transport by adjusting the ratio of lattice parameters, \(d_A/d_B\), in the various sequences. Next, the influences of the incidence angle, \(\theta_0\), on the transmission spectra are also studied. Obviously, the zero-\(\bar{k}\) gap associated with new Dirac point is insensitive to the incidence angle, as shown in figure 4. In contrast, the Bragg gap shifts upwards in energy as the incidence angle increases. Compared with the weak dependence of zero-\(\bar{k}\) gap on the incidence angles, the Bragg gaps change sensitively with respect to incidence angle \(\theta_0\).

Additionally, the multi-Dirac-points could appear in the GSL with periodic [9, 15] and aperiodic [20] structures. Figure 5(a) demonstrates that the extra Dirac points located at \(k_y \neq 0\) can also emerge in the GSL of the DP sequence, where \(k_y = 0.01\) nm\(^{-1}\) and \(d_A/d_B = 1\). We show the energy band gaps versus the lattice constants in the case of \(d_A = d_B = d\). The zero-\(\bar{k}\) gap, associated with the multi-Dirac-points, oscillates with changing the lattice constants, thus open and close periodically, while the other Bragg gaps are significantly shifted. Actually, the existence of multi-Dirac-points can be explicitly explained by equations (4) and (5). It is seen from equation (4) that when the values of \(3q_A d_A\)
where \( \text{band structures in both cases, as shown in figures 5} \)
and \(-q_B d_B\) approach to the value of \(m\pi\), the slope of the band edges near the new Dirac point becomes smaller. Furthermore, when the condition \(3q_A d_A = -q_B d_B = m\pi\) \(8\)
is fulfilled, we have \(\sin(3q_A d_A) = \sin(q_B d_B) = 0\) in equation \(5\), so that the zero-\(\vec{k}\) gap will be closed and a pair of new zero-averaged wave-number states emerges at \(k_y \neq 0\) (see figure 5(c)). As a result, in the case of \(3q_A d_A = -q_B d_B < \pi\), there is only one Dirac point happened at \(k_y = 0\), whereas the additional Dirac points will occur in pairs at \(k_y \neq 0\), when the condition \(3q_A d_A = -q_B d_B = m\pi\) is satisfied. However, figures 5(a) and (d) illustrate the multi-Dirac-points in the DP sequence are different from those in the TM sequence. To compare them, we choose \(S_2 = ABAA\) for DP and \(S_2 = ABB\) for the TM sequence and plot the electronic band structures in both cases, as shown in figures 5(c) and (d).

We see from figure 5(a) that the multi-Dirac-points appear at the same energy, \(E = 36.4\) meV, which is different from the location, \(E = 37.5\) meV, of Dirac point for \(k_y = 0\). Moreover, the energy corresponding to the multi-Dirac-points in DP sequence will be close to \(E = 37.5\) meV, when \(k_y \rightarrow 0\). However, as shown in figures 5(b) and (d), the Dirac point for \(k_y = 0\) and multi-Dirac-points for \(k_y \neq 0\) happen at the same energy \(E = 25\) meV in the TM sequence with \(\tau_n = 1\), because the condition for the existence of multi-Dirac-points should be modified as \(2q_A d_A = -2q_B d_B = m\pi\) in this case. It tells us that though the total numbers of layer \(A\) and \(B\) are the same for the TM and DP sequences, the behaviours of multi-Dirac-points in TM and DP sequences are totally different, because the ratio, \(\tau_n = N_A/N_B\), is not equal.

Regarding the electronic transport, the total conductance and the Fano factor are also interesting. In figure 6, we calculate the total conductance \(G/G_0\) and the Fano factor \(F\) in quasi-periodic GSL of DP sequence, \((ABAA)^2\). Again, we have found several unique features associated with new Dirac point and zero-\(\vec{k}\) gap, as shown in figure 6. Firstly, the curve of angular-averaged conductance reaches its minimum at the Dirac point, and forms a liner cone around Dirac point. Meanwhile the Fano factor reaches the value of 1/3 approximately \([30]\). Secondly, the conductance and the Fano factor will shift with adjusting the ratio of \(d_A/d_B\). Actually, this will be useful to modulate the conductance of such GSL by changing the ratio of lattice constants.

Finally, what we should mention is that the transmission spectrum and corresponding electronic transport properties including conductance and the Fano factor in the DP sequence are quite different from those in FB and TM sequences. To clarify it, we shall compare the Dirac point in three different sequences. In figure 7, we present the location of Dirac point versus the variable order \(n\) in FB, TM and DP sequences. In TM sequences, the location of new Dirac point does not depend on the order \(n\), because the numbers of layer \(A\) and \(B\) are the same as mentioned above. As for FB and DP, the numbers of layer \(A\) and \(B\) are different in each order \(n\) \((n > 1)\). As a consequence, the location of Dirac point depends on the variable order \(n\), but it will become stable for \(n \gg 1\), since the ratio of numbers of layer \(A\) and \(B\), \(N_A/N_B\), tends to \(\tau_n = (1 + \sqrt{5})/2\) for the FB sequence \([19, 27]\) and \(\tau_n = 2\) roughly for DP sequence \([27]\).

In the limit of an infinite sequence, the ratio of numbers of layer \(A\) and \(B\) for FB, TM and DP sequences can be systematically understood in terms of trace maps in \([26]\). The difference...
on new Dirac points in various sequences is quite natural, because the physical origin of zero-\(\bar{\hat{k}}\) gap is the total zero phase, suggested by equation (6).

4. Summary

To summarize, we have studied the electronic band gap and transport in GSL of the DP sequence using the transfer matrix method. We have found that the Dirac point, multi-Dirac-points and associated zero-\(\bar{\hat{k}}\) gaps have emerged in such a quasi-periodic structure. The zero-\(\bar{\hat{k}}\) gap and Dirac point are robust against the lattice constants and incidence angle. The results are also compared with those in GSL of FB and TM sequences. We hope that all these results may lead to applications in the control of electron transport in GSLs.

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