Periodic Landau gauge and Quantum Hall effect in twisted bilayer graphene

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I. INTRODUCTION

Two dimensional electron systems are realized in graphene. Bilayer graphene and twisted bilayer graphene have been shown to have many interesting properties and been studied extensively. The quantum Hall effects in single layer graphene and bilayer graphene are well understood by the energy versus magnetic field, which is known as the Hofstadter butterfly diagram, in the tight binding models of honeycomb net and Bernal-stacked bilayer graphene. The quantized value of the Hall conductance is obtained by the solution of the Diophantine equation. Since a supercell can be large, magnetic flux through a supercell normalized by the flux quantum can be a fractional number with a small denominator, even when a magnetic field is not extremely strong. As a result, quantized Hall conductance can be a solution of the Diophantine equation which cannot be obtained by the approximation of the linearized energy dispersion near the Dirac points.

Energy versus magnetic field (Hofstadter butterfly diagram) in twisted bilayer graphene is studied theoretically. If we take the usual Landau gauge, we cannot take a finite periodicity even when the magnetic field through a supercell is a rational number. We show that the periodic Landau gauge, which has the periodicity in one direction, makes it possible to obtain the Hofstadter butterfly diagram. Since a supercell can be large, magnetic flux through a supercell normalized by the flux quantum can be a fractional number with a small denominator, even when a magnetic field is not extremely strong. As a result, quantized Hall conductance can be a solution of the Diophantine equation which cannot be obtained by the approximation of the linearized energy dispersion near the Dirac points.

m₁ = 2, m₂ = 1, L₁ = m₁ a₁ + m₂ a₂

FIG. 1. (color online). Twisted bilayer graphene with (m₁, m₂) = (2, 1). Large (small) open and filled circles are A and B sublattice in the first (second) layer, respectively. The second layer is rotated by π/3 - α. The orange area is the supercell.

Solution of the Diophantine equation Eq. (24) with sᵣ = 1 (sᵣ = 2) in single layer (bilayer) graphene.

Twisted bilayer graphene attracts much attention recently. When two layers are twisted in a commensurate way, a supercell becomes large with a moiré pattern (if a usual Landau gauge is used in that system, only magnetic flux through a supercell is allowed). String gauge, which is obtained by adding periodic boundary conditions in the presence of the uniform magnetic field, has been introduced to study the periodic system in a magnetic field. The periodic vector potential (equivalent to the periodic Landau gauge) has been introduced to study the Schrödinger equation which cannot be obtained by the approximation of the linearized energy dispersion near the Dirac points.

When we use the usual Landau gauge in twisted bilayer graphene with long range hoppings, there are no periodicity in the phase factor of hoppings. In that case we cannot obtain the Hofstadter butterfly diagram. In this paper we show that we can recover the periodicity when a magnetic flux through a supercell is a rational number, if we use the periodic Landau gauge. As far as we know, a special choice of gauge was first used to study the system of the 4 × 4 square lattice with periodic boundary conditions in the presence of the uniform magnetic flux p/16 with p = 1, 2, 3, · · · 24 (if a usual Landau gauge is used in that system, only magnetic flux p/4 is allowed). String gauge, which is obtained by adding the flux line with a flux quantum, has been introduced to study the periodic system in a magnetic field. The periodic vector potential (equivalent to the periodic Landau gauge) has been introduced to study the Schrödinger equation.
II. TWISTED BILAYER GRAPHENE

In a unit cell in each layer there are two sites, A and B, which form triangular lattices respectively. We define unit vectors as

\[ \mathbf{a}_1 = a \left( \frac{\sqrt{3}}{2}, -\frac{1}{2} \right), \tag{1} \]

and

\[ \mathbf{a}_2 = R_{\pi/3} \mathbf{a}_1 = a \left( \frac{\sqrt{3}}{2}, \frac{1}{2} \right), \tag{2} \]

where \( a \) is the lattice constant and \( R_{\pi/3} \mathbf{a}_1 \) is the \( \pi/3 \) rotated vector of \( \mathbf{a}_1 \). Hereafter we take \( a = 1 \) for simplicity. The reciprocal lattice vectors are given by

\[ \mathbf{G}_1 = 2\pi \left( \frac{1}{\sqrt{3}}, -1 \right), \tag{3} \]

\[ \mathbf{G}_2 = 2\pi \left( \frac{1}{\sqrt{3}}, 1 \right). \tag{4} \]

In the first layer, sites in the A sublattice are given by sets of two integers \((j_1, j_2)\) as

\[ r^A_{j_1,j_2} = j_1 \mathbf{a}_1 + j_2 \mathbf{a}_2. \tag{5} \]

Three vectors connecting nearest neighbor sites in the first layer are

\[ \mathbf{\delta}_a = \left( \frac{\sqrt{3}}{2}, 0 \right), \tag{6} \]

\[ \mathbf{\delta}_b = \left( -\frac{\sqrt{3}}{2}, 0 \right), \tag{7} \]

\[ \mathbf{\delta}_c = \left( 0, -\frac{1}{2} \right). \tag{8} \]

Sites in the B sublattice in the first layer are given by

\[ r^B_{j_1,j_2} = r^A_{j_1,j_2} + \mathbf{\delta}_a. \tag{9} \]

The AB (Bernal) stacking of bilayer graphene is obtained by rotating the second layer around one of the A site in the first layer by the angle \((2n + 1)\pi/3\), where \( n \) is an integer. In this case the A sublattice in the second layer is just above the A sublattice in the first layer, but the B sublattice in the second layer is on the center of the hexagon in the first layer. The same stacking is obtained by translating the second layer by \(-\mathbf{\delta}_a, -\mathbf{\delta}_b\) or \(-\mathbf{\delta}_c\). When the rotation angle is \(2n\pi/3\), we obtain the AA stacking, i.e., all sites in the second layer are on the sites in the first layer. We obtain twisted bilayer graphene, when the rotation angle is neither \((2n + 1)\pi/3\) nor \(2n\pi/3\).

When twisted bilayer graphene has supercell with finite number of sites, it is called commensurate twisted bilayer graphene. We construct commensurate twisted bilayer graphene as follows: Since there is six-fold symmetry in twisted bilayer graphene, we can take a supercell as a diamond with the angle \(\pi/3\) as shown in Fig. 1. We define unit vectors of superlattice with two integers \(m_1\) and \(m_2\) \((m_1 \neq 0, m_2 \neq 0, \text{ and } |m_1| \neq |m_2|)\):

\[ \mathbf{L}_1 = r^A_{m_1,m_2} = m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2, \tag{10} \]

\[ \mathbf{L}_2 = R_{\pi/3} \mathbf{L}_1 = r^A_{-m_2,(m_1+m_2)}. \tag{11} \]

Twisted bilayer graphene with \((m_1, m_2) = (2, 1)\) is shown in Fig. 1. Since

\[ \mathbf{a}_1 \cdot \mathbf{a}_2 = \frac{1}{2}, \tag{12} \]

we obtain

\[ |\mathbf{L}_1|^2 = |\mathbf{L}_2|^2 = m_1^2 + m_2^2 + m_1 m_2 \equiv n_0. \tag{13} \]

The area of a supercell is given by

\[ S = |\mathbf{L}_1||\mathbf{L}_2| \sin \frac{\pi}{3} = \frac{\sqrt{3}}{2} n_0. \tag{14} \]

There is another site in the supercell that has the same distance from the origin as \(|\mathbf{L}_1|\), which we define \(\mathbf{L}'_1\) as shown in Fig. 1

\[ \mathbf{L}'_1 = r^A_{m_2,m_1} = m_2 \mathbf{a}_1 + m_1 \mathbf{a}_2. \tag{15} \]
We define $\alpha$ by the angle between the vectors $\mathbf{L}'_1$ and $\mathbf{L}_1$. Since
\[ \mathbf{L}'_1 \cdot \mathbf{L}_1 = \frac{1}{2}(m_1^2 + 4m_1m_2 + m_2^2), \]
we obtain
\[ \cos \alpha = \frac{\mathbf{L}'_1 \cdot \mathbf{L}_1}{|\mathbf{L}'_1||\mathbf{L}_1|} = \frac{m_1^2 + 4m_1m_2 + m_2^2}{2(m_1^2 + m_1m_2 + m_2^2)}. \]

Then we obtain twisted bilayer graphene by rotating the second layer with the angle $\pi/3 - \alpha$ to move the vector $\mathbf{L}'_1$ into $\mathbf{L}_2$. We obtain another type of twisted bilayer graphene when we rotate the second layer by the angle $-\alpha$. In this paper we take the rotation angle $\pi/3 - \alpha$ to obtain the Bernal stacking when $\alpha \to 0$.

The Bravais lattice of twisted bilayer graphene is the $-\alpha/2$-tilted two-dimensional triangular lattice with the primitive vectors $\mathbf{L}_1$ and $\mathbf{L}_2$. A supercell has $n_0$ sites in A and B sublattice in each layer, hence $4n_0$ sites.

### III. TIGHT BINDING MODEL AND PERIODIC LANDAU GAUGE

We consider tight binding models in a uniform magnetic field. Spin is not taken into account. When a magnetic field is applied, the hopping $t_{ij}$ between sites $\mathbf{r}_i$ and $\mathbf{r}_j$ ($\mathbf{r}_i$ and $\mathbf{r}_j$ are on the same layer or on different layers) has the factor $\exp(i\theta_{ij})$ with a phase $\theta_{ij}$ given by
\[ \theta_{ij} = \frac{2\pi}{\phi_0} \int_{\mathbf{r}_i}^{\mathbf{r}_j} \mathbf{A} \cdot d\mathbf{r}, \]
where $\mathbf{A}$ is a vector potential and
\[ \phi_0 = \frac{eh}{c}, \]
is the flux quantum with charge $e$, the speed of light $c$ and the Planck constant $h$. The Hamiltonian is
\[ \mathcal{H} = -\sum_{\langle i,j \rangle}(e^{i\theta_{ij}} c^\dagger_i c_j + h.c.), \]
where $c^\dagger_i$ and $c_i$ are the creation and annihilation operators at site $i$, respectively. We take the approximation.

\[
\begin{align*}
    t_{ij} &= \begin{cases}
        t \exp \left( \frac{-d - |\delta_a|}{\delta} \right), & \text{if sites } i \text{ and } j \text{ are on the same layer}, \\
        t_{12} \exp \left( \frac{-d - d_0}{|\delta_{12}|} \right), & \text{if sites } i \text{ and } j \text{ are on different layers}
    \end{cases},
\end{align*}
\]
where $d = |\mathbf{r}_i - \mathbf{r}_j|$ is the distance between sites $i$ and $j$ and $d_0$ is the distance between layers. When we take $\delta \to 0$ and $t_{12} = 0$, we obtain two independent layers of honeycomb lattice with only nearest-neighbor hoppings. When $t_{12}$, $\delta$ and $\delta_{12}$ are finite, we obtain twisted bilayer graphene with finite range hoppings. Interlayer hoppings are not restricted to the perpendicular direction.

The energy is independent of the sign of the interlayer hoppings $t_{12}$, since we obtain the same Hamiltonian by changing the sign of $t_{12}$, and the signs of $c^\dagger_i$ and $c_i$ in the second layer simultaneously.

Even if the flux per supercell is an integer times the flux quantum $\phi_0$, the phase factor $\theta_{ij}$ is not periodic with modulus $2\pi$, in which case we use the usual Landau gauge ($\mathbf{A} = H_{x,y}$). For single layer graphene with only nearest-neighbor hoppings, we could take a special gauge in which the phase factor appears only in the links for one of the three directions, $\delta_a$, $\delta_b$ or $\delta_c$. However, such choice of gauge is not possible for twisted bilayer graphene.

In this paper we study the energy spectrum in the twisted bilayer graphene in magnetic field by using the periodic Landau gauge, which is essentially the same as the gauge used by Nemec and Cuniberti to study the Bernal stacked bilayer graphene. We explain the periodic Landau gauge for the square lattice in Appendix A.

The generalization to the non-square lattice is given in Appendix B.

When flux through a supercell is
\[ \Phi = SH = \frac{p}{q} \phi_0, \]
where $p$ and $q$ are mutually prime integers in twisted bilayer graphene with commensurate twisted angle (Eq. (17)), energy spectrum is obtained by the eigenvalues of $(4n_0q) \times (4n_0q)$ matrix, as in the case of the single layer graphene where it is obtained by the eigenvalues of $(2q) \times (2q)$ matrix.

In Figs. 2, we plot the energy versus magnetic flux through a unit cell in each layer with only nearest-neighbor hoppings. In Figs. 3, 4 and 5 we take parameters for the bilayer graphene $t = 2.7$ eV, $t_{12} = -0.48$ eV ($t_{12}/t = -0.18$), $|\delta_a| = 0.142$ nm, $d_0 = 0.335$ nm, and $\delta = \delta_{12} = 0.0453$ nm ($|\delta|/|\delta_a| = 0.184$), and we plot the energy versus magnetic flux through a unit cell in each layer ($\phi = \Phi/n_0$) in twisted bilayer graphene.

### IV. DIOPHANTINE EQUATION

Consider the case
\[ \frac{\Phi}{\phi_0} = \frac{p}{q}, \]
where $\Phi$ is the flux through a supercell, $p$ and $q$ are integers. In square lattice and honeycomb lattice $\Phi = \phi$, and in twisted bilayer graphene $\Phi = n_0\phi$, where $\phi$ is the flux through a unit cell in each layer. When chemical potential is in the $r$th gap from the bottom, we have the Diophantine equations
\[ r = qs_r + pt_r, \]
where $s_r$ and $t_r$ are integers.
FIG. 2. (color online). Energy spectrum in single layer graphene with only nearest-neighbor hoppings. Numbers in the figures are \((s_r, t_r)\). Quantized value of Hall conductance is given by \(t_r\). See Eqs. (24) and (25).

which gives quantized Hall conductance by

\[ \sigma_{xy} = \frac{e^2}{h} t_r. \]  \hspace{1cm} (25)

If we take account of the spin and neglect the Zeeman energy, the Hall conductance is multiplied by 2.

For the tight binding models with only nearest-neighbor hoppings in square lattice or honeycomb lattice, the flux quantum \(\phi_0\) through a unit cell is equivalent to zero magnetic flux. As a result, the energy spectrum is periodic with respect to \(\phi\) with a period \(\phi_0\). Even when we consider the models with long range hoppings, the energy spectra are periodic function of \(\phi\) with a period \(2\phi_0\) or \(6\phi_0\) in the square lattice or the honeycomb lattice, respectively. This is because the smallest areas enclosed by hoppings are \(1/2\) and \(1/6\) of the areas of a unit cell in the square lattice and the honeycomb lattice, respectively. See Fig. 6 for the honeycomb lattice. The energy spectrum is also periodic with respect to \(\phi\) with a period \(6\phi_0\) for Bernal stacked bilayer graphene. The situation is drastically changed in twisted bilayer graphene. When there are hoppings between layers in twisted bilayer graphene, projected areas enclosed by hoppings have irrational values as shown in the red triangles in Fig. 6. As a result the energies are not periodic in \(\phi\).

In single layer graphene, there are \(2q\) band when flux through a supercell is \((p/q)\phi_0\). In Fig. 2 we show \((s_r, t_r)\) for several gaps for single layer graphene. Large gaps have indices \(t_r = 0, 1, 2\), and \(2\). The gaps, which are focused at the bottom of the band at \(\phi \to 0\), have \(s_r = 2\), and \(t_r = 1, 2, 3, \ldots\). They correspond to the usual Landau levels. The gaps, which are focused at the top of the band at \(\phi \to 0\), have \(s_r = 2\), and \(t_r = -1, -2, -3, \ldots\). The gaps near half filling \((E \approx 0)\) and \(\phi \ll \phi_0\) have \(s_r = 1\) and \(t_r = \pm 1, \pm 3, \pm 5, \ldots\), which have been observed in graphene. For the finite \(\phi\) the band near \(E \approx 0\) becomes broadened gradually and many gaps can be seen in Fig. 2. Note that \(\phi = \phi_0\) in a unit cell corresponds

FIG. 3. (color online). Energy spectrum in twisted bilayer graphene with \((m_1, m_2) = (3, 2)\). Numbers in the figures are \((s_r, t_r)\). Quantized value of Hall conductance is given by \(t_r\).
FIG. 4. (color online). Energy spectrum in twisted bilayer graphene with \((m_1, m_2) = (8, 7)\). Numbers in the figures are \((s_r, t_r)\). Quantized value of Hall conductance is given by \(t_r\).

To 40,000 T, which is not attainable in a present day laboratory.

In Figs. 3, 4, and 5, we plot the Hofstadter butterfly diagrams for twisted bilayer graphene with \((m_1, m_2) = (3, 2)\), \((8, 7)\) and \((12, 11)\), respectively. Although energy gaps near the bottom have \(s_r = 0\) and \(t_r = 1, 2, 3, \cdots\), for all three cases as in single layer graphene, there are crossings of the bands near the bottom of the energy. For example, the gap indexed by \((0, 2)\) vanishes at \(\phi/\phi_0 \approx 0.16\) and \(E/t \approx -2.8\), at which band-crossing occurs. These crossings of bands can be understood by the independent Landau levels for the two local minimums of the energy in the absence of a magnetic field (see Fig. 7).

Near the top of the energy the large gaps are indexed by \((s_r, t_r) = (4n_0, -2), (4n_0, -4), (4n_0, -6), \cdots\), which can be understood by the fact that there are \(4n_0\) bands and nearly degenerate two local maxima of the energy in the absence of a magnetic field.

A very interesting feature is seen near half filling. Besides the large gaps of \((s_r, t_r) = (2n_0, \pm 2)\), many new gaps become visible as \(\alpha\) becomes small. For example, \((s_r, t_r) = (2n_0 - 2, 0), (2n_0 - 2, \pm 2), (2n_0 + 2, \pm 2), (2n_0 - 2, \pm 2), \cdots\) are seen in the lower figures in Figs. 4 and 5. These new gaps are caused by a large supercell, which has \(4n_0\) sites. Since Hall conductance is given by \(t_r\), the band between the gaps with same \(t_r\) \((2n_0, 2)\) and \((2n_0 - 2, 2)\), for example) does not contribute to the Hall conductance. Mathematically, that band is a Cantor set and consists of narrower bands and much smaller gaps. Each narrow band gives a finite Hall conductance and the total contribution vanishes.

V. SUMMARY

We obtain the Hofstadter butterfly diagram for twisted bilayer graphene. The use of the periodic Landau gauge is crucial. Due to large number of sites \((4n_0)\) in a supercell, a rich structure of the Hofstadter butterfly di-
FIG. 6. (color online). Twisted bilayer graphene. When there are only nearest-neighbor hoppings in each layer, an area enclosed by hoppings is $S$ (blue hexagon). When there are second-nearest-neighbor or third-nearest-neighbor hoppings in each layer, areas enclosed by hoppings are $S/6$ and its multiples (blue triangle). The hoppings between layers make the area enclosed by hoppings to be irrational number times $S$ (red triangles).

FIG. 7. (color online). Schematic band structure near the bottom of the energy. There are two local minimums and nearly independent Landau Levels (dashed blue lines and solid red lines).

FIG. 8. (color online). The $y$ component of vector potentials for Landau gauge ($A_y^{(L)}$, dashed line) and periodic Landau gauge ($A_y^{(pL)}$, thick blue line) for the square lattice.
We can obtain other vector potential by gauge transformation, i.e., adding $\nabla \chi(r)$ to $A$. It is crucial to have periodicity in a gauge of twisted bilayer graphene. We take

$$\chi(r) = -H [x, y], \quad (A3)$$

and so,

$$A^{(pL)}(x, y) = H (x\hat{y} - \nabla (|x| y))$$

$$= H \left( (x - |x|)\hat{y} - y \sum_{n=-\infty}^{\infty} \delta(x - n + \epsilon) \hat{x} \right), \quad (A4)$$

where $\epsilon$ is an infinitesimal and $|x|$ is the floor function (largest integer not greater than $x$), i.e., $x - |x|$ is the fractional part of $x$. In this gauge, which we call the periodic Landau gauge, $A^{(pL)}$ is periodic with respect to $x$ with period 1, as shown in Fig. 8. In order to make $A_y^{(pL)}$ be periodic in the $y$ direction $A_y^{(pL)}$ is a discontinuous function of $x$ as shown in Fig. 8 and $A_x^{(pL)}$ is the sum of delta functions. These singular functions do not cause any problems. We have no ambiguity in the phase factor $\theta_{ij}$, since we have added the infinitesimal $\frac{2\pi}{pL}$.

Note that $A_y^{(pL)}$ depends on $y$ and it is not periodic in the $y$ direction. However, the dependence of $y$ in $A^{(pL)}$ appears always with the delta function, so $\exp(i\theta_{ij})$ is periodic in the $y$ direction, as we show below.

The difference of the usual Landau gauge and the periodic Landau gauge is seen in Fig. 9 in which a uniform magnetic field with $(p/q)\phi_0$ through a unit cell is applied to square lattice. If we take the usual Landau gauge, the phase factor is zero except vertical links as shown in Fig. 9 (a). The phase factor for the vertical links at $x = n$ is $\theta_{ij} = 2\pi p/n q$. The periodicity in the $x$ direction is $q$ times larger than the periodicity in the absence of a magnetic field. However, if there are other sites in a unit cell, the periodicity of the system is changed (this is the case in twisted bilayer graphene, where there are $4n_0$ sites in the supercell (see Figs. 1 and 6)). In order to demonstrate it in the square lattice, we add sites at $(n + \gamma_1, m), (n, m + \gamma_2)$, and at $(n + \gamma_1, m + \gamma_2)$, where $n$ and $m$ are integers, $0 < \gamma_1 < 1$ and $0 < \gamma_2 < 1$ (filled green circles). Blue letters are flux in rectangles. The system is periodic only when $\gamma_2$ is a rational number. (c) The phases (beside arrows) and the flux through rectangles (blue letters) in the periodic Landau gauge. The system is periodic in the $x$ direction with period 1 and in the $y$ direction with period $q$.

FIG. 9. (color online). (a) The numbers beside the arrows are the phases in the usual Landau gauge for the square lattice with flux $(p/q)\phi_0$ in a unit cell. The system is periodic in the $x$ direction with period $q$. (b) Sites are added at $(n + \gamma_1, m), (n, m + \gamma_2)$, and $(n + \gamma_1, m + \gamma_2)$, where $n$ and $m$ are integers, $0 < \gamma_1 < 1$ and $0 < \gamma_2 < 1$ (filled green circles). Blue letters are flux in rectangles. The system is periodic only when $\gamma_2$ is a rational number. (c) The phases (beside arrows) and the flux through rectangles (blue letters) in the periodic Landau gauge. The system is periodic in the $x$ direction with period 1 and in the $y$ direction with period $q$. The periodicity is recovered by taking the periodic Landau gauge (Eq. (A3)). The periodicity is 1 in the $x$ direction, since $A^{(pL)}$ is periodic in the $x$ direction. The delta functions in Eq. (A3) make the nonzero phases for the horizontal links as shown by thick red horizontal arrows in Fig. 9(c). The magnetic flux through each small rectangles is obtained by the sum of the surrounding phases $\theta_{ij}$ and it is proportional to the area. The phase factor for the horizontal link between $r_i = (n, m)$ and $r_j = (n + 1, m)$ is $\theta_{ij} = -2\pi n \gamma_2 p/q$. If $\gamma_2$ is an irrational number, $\exp(i\theta_{ij})$ cannot be periodic with respect to $x$. The periodicity is recovered by taking the periodic Landau gauge (Eq. (A4)). The periodicity is 1 in the $x$ direction, since $A^{(pL)}$ is periodic in the $x$ direction. The delta functions in Eq. (A3) make the nonzero phases for the horizontal links as shown by thick red horizontal arrows in Fig. 9(c). The magnetic flux through each small rectangles is obtained by the sum of the surrounding phases $\theta_{ij}$ and it is proportional to the area. The phase factor for the horizontal link between $r_i = (n, m)$ and $r_j = (n + 1, m)$ is $\theta_{ij} = -2\pi n \gamma_2 p/q$. If $\gamma_2$ is an irrational number, $\exp(i\theta_{ij})$ cannot be periodic with respect to $x$.
Appendix B: periodic Landau gauge in non-square lattice

The periodic Landau gauge discussed in Appendix A is generalized to non-square two-dimensional lattices, which have primitive vectors of the supercell \( L_1 \) and \( L_2 \), which are not orthogonal. The reciprocal lattice vectors are

\[
F_1 = 2\pi \frac{L_2 \times \hat{z}}{(L_1 \times L_2) \cdot \hat{z}},
\]

and

\[
F_2 = 2\pi \frac{\hat{z} \times L_1}{(L_1 \times L_2) \cdot \hat{z}}.
\]

We define oblique coordinate system \((\xi_1, \xi_2)\) by

\[
r = \left( \begin{array}{c} x \\ y \end{array} \right) = \xi_1 L_1 + \xi_2 L_2,
\]

where \(x\) and \(y\) are the coordinates in an orthogonal system. For twisted bilayer graphene we have

\[
\xi_1 = \frac{1}{n_0} \left( \frac{\sqrt{3}}{3} (m_1 + 2m_2)x - m_3 y \right),
\]

\[
\xi_2 = \frac{1}{n_0} \left( \frac{\sqrt{3}}{3} (m_1 - m_2)x + (m_1 + m_2)y \right).
\]

The reciprocal vectors are

\[
F_1 = \frac{m_1 + m_2}{n_0} G_1 + \frac{m_2}{n_0} G_2,
\]

and

\[
F_2 = \frac{-m_2}{n_0} G_1 + \frac{m_1}{n_0} G_2.
\]

The Landau gauge for the oblique coordinate system is

\[
A^{(L,\text{nsq})} = \frac{SH}{2\pi} \xi_1 F_2,
\]

which is a generalization of Eq. (A2) to the non-square lattice. To make the vector potential periodic with respect to \( \xi_1 \), we take the periodic Landau gauge as

\[
A^{(pL,\text{nsq})} = \frac{SH}{2\pi} \left( (\xi_1 - |\xi_1|) F_2 - \xi_2 \sum_{n=1}^{\infty} \delta(\xi_1 - n + \epsilon) F_1 \right).
\]

In Fig. 10 we show an example of \( \theta_{ij} \) between the nearest neighbor sites in the first layer for \( m_1 = 2, m_2 = 1 \) (\( n_0 = 7 \)) and the flux through a supercell is \( \phi_0 \) (\( p/q = 1/1 \)). Note that the phase factor \( \theta_{ij} \) crossing the line \( \xi_1 = n \) (red numbers in Fig. 10) is not periodic in the \( L_2 \) direction but \( \exp(i\theta_{ij}) \) is periodic.

The advantage of taking the periodic Landau gauge is that the vector potential \( A \) is periodic in \( \xi_1 \) with period 1. This ensures the periodicity of the system in \( L_1 \) direction. The system has a periodicity in the \( L_2 \) direction if the flux per supercell is an rational number times \( \phi_0 \).

If the flux per a supercell is a rational number \( p/q \), i.e.

\[
\Phi = n_0 \phi = SH = \frac{p}{q} \phi_0,
\]

the phase factor \( \theta_{ij} \) in Eq. (18) with the periodic Landau gauge (Eq. (B9)) has the same value when \( r_i \) and \( r_j \) are translated by \( L_1 \). It has also the same value when \( r_i \) and \( r_j \) are translated by \( L_2 \) if the link connecting \( r_i \) and \( r_j \) does not cross the line \( \xi_1 = n \), where \( n \) is an integer. If the link connecting \( r_i \) and \( r_j \) crosses the line \( \xi_1 = n \), \( \theta_{ij} \) increases by \( \pm 2\pi p/q \) when \( r_i \) and \( r_j \) are translated by \( L_2 \) (\( \pm \) depends on the sign of \( F_1 \cdot \hat{d} \)). Therefore periodicity must be \( q \) times larger in the \( L_2 \) direction.

FIG. 10. (color online). The first layer of twisted bilayer graphene with \((m_1, m_2) = (2, 1)\) \((n_0 = 7)\). The numbers on the links between the nearest neighbors in units of \(2\pi/(18n_0^2) = 2\pi/882\) when the flux per supercell is \( \phi_0 \), i.e. the flux per unit hexagon is \( \phi_0/n_0 \) (we obtain \(4 - (-35) + 242 - 34 - (-155) - 148) \times 2\pi/882 = 2\pi/7\), for example). We take the periodic Landau gauge (Eq. (18)). The contribution from the delta function in Eq. (B9) is finite for the red numbers, while it is zero for the blue numbers.
1. K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jaing, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, Science 306, 666 (2004).
2. E. McCann and V. I. Fal’ko, Phys. Rev. Lett. 96, 086805 (2006).
3. S. Shallcross, S. Sharma, E. Kandelaki, and O. A. Pankratov, Phys. Rev. B 81, 165105 (2010).
4. K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, and A. A. Firsov, Nature 438, 197 (2005).
5. Y. Zhang, Y.-W. Tan, H. L. Stormer, and P. Kim, Nature 438, 201 (2005).
6. Y. Hasegawa and M. Kohmoto, Phys. Rev. B 74, 155415 (2006).
7. Y. Hatsugai, T. Fukui, and H. Aoki, Phys. Rev. B 74, 205414 (2006).
8. P. Dietl, F. Piéchon, and G. Montambaux, Phys. Rev. Lett. 100, 236405 (2008).
9. N. Nemec and G. Cuniberti, Phys. Rev. B 75, 201404 (2007).
10. D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. 49, 405 (1982).
11. M. Kohmoto, Annals of Physics 160, 343 (1985).
12. M. Kohmoto, Phys. Rev. B 39, 11943 (1989).
13. J. M. B. Lopes dos Santos, N. M. R. Peres, and A. H. Castro Neto, Phys. Rev. Lett. 99, 256802 (2007).
14. J. Hass, F. Varchon, J. E. Millán-Otoya, S. Spear, N. Sharma, W. A. de Heer, C. Berger, P. N. First, L. Magaud, and E. H. Conrad, Phys. Rev. Lett. 100, 125504 (2008).
15. S. Shallcross, S. Sharma, and O. A. Pankratov, Phys. Rev. Lett. 101, 056803 (2008).
16. E. J. Mele, Phys. Rev. B 81, 161405 (2010).
17. G. Trambly de Laissardière, D. Mayou, and L. Magaud, Nano Letters 10, 804 (2010).
18. R. Bistritzer and A. H. MacDonald, Proceedings of the National Academy of Sciences 108, 12233 (2011).
19. L. A. Ponomarenko, R. V. Gorbachev, G. L. Yu, D. C. Elias, R. Jalil, A. A. Patel, A. Mishchenko, A. S. May- orov, C. R. Woods, J. R. Wallbank, M. Mucha-Kruczyński, B. A. Piot, M. Potemski, I. V. Grigorieva, K. S. Novoselov, F. Guinea, V. I. Fal’ko, and A. K. Geim, Nature (London) 497, 594 (2013).
20. C. R. Dean, L. Wang, P. Maher, C. Forsythe, F. G. and Y. Gao, J. Katoch, M. Ishigami, P. Moon, M. Koshino, T. Taniguchi, K. Watanabe, K. L. Shepard, J. Hone, and P. Kim, Nature (London) 497, 598 (2013).
21. D. S. Lee, C. Riedl, T. Beringer, A. H. Castro Neto, K. von Klitzing, U. Starke, and J. H. Smet, Phys. Rev. Lett. 107, 216602 (2011).
22. R. Bistritzer and A. H. MacDonald, Phys. Rev. B 84, 035440 (2011).
23. P. Moon and M. Koshino, Phys. Rev. B 85, 195458 (2012).
24. Z. F. Wang, F. Liu, and M. Y. Chou, Nano Letters 12, 3833 (2012).
25. D. Poilblanc, Y. Hasegawa, and T. M. Rice, Phys. Rev. B 41, 1949 (1990).
26. Y. Hatsugai, K. Ishibashi, and Y. Morita, Phys. Rev. Lett. 83, 2246 (1999).
27. A. Trellakis, Phys. Rev. Lett. 91, 056405 (2003).
28. W. Cai and G. Galli, Phys. Rev. Lett. 92, 186402 (2004).
29. T. Nakazishi and T. Ando, Journal of the Physical Society of Japan 70, 1647 (2001).
30. J.-W. Rhim and K. Park, Phys. Rev. B 86, 235411 (2012).
31. M. Sato, D. Tobe, and M. Kohmoto, Phys. Rev. B 78, 235322 (2008).