Circular quantum dots in twisted bilayer graphene
M. Mirzakhani, F. M. Peeters, and M. Zarenia
Phys. Rev. B 101, 075413 — Published 11 February 2020
DOI: 10.1103/PhysRevB.101.075413
Circular quantum dots in twisted bilayer graphene

M. Mirzakhani, F.M. Peeters, and M. Zarenia

1 School of Physics, University of the Witwatersrand, P.O. Box Wits, Johannesburg, South Africa
2 Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium
3 Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA

(Dated: January 29, 2020)

PACS numbers: 81.05.ue, 73.22.Pr, 73.21.La

I. INTRODUCTION

Over the past year, twisted bilayer graphene (tBLG), i.e., BLG with relative twist between its two coupled graphene layers, has been the subject of intensive theoretical and experimental research works. The main interest results from the new discovery of superconductivity and correlated insulating phases in tBLG at a so-called magic twist angle. It is fascinating that with a small twist angle between the two layers of BLG, the electronic and transport properties of the system undergo profound changes. In this paper, we aim to investigate the effect of twisting angle on the energy levels of a circular QD in tBLG. QDs have been studied extensively in different two-dimensional (2D) materials, i.e., monolayer, bilayer, and few-layer graphene, transition metal dichalcogenides, hexagonal boron nitride, phosphorene, etc.

Among QDs in 2D materials, graphene-based QDs (geometry or gate induced) with desirable properties for applications have been received particular interest. The studies show that the electronic and optical properties of graphene QDs can be tuned by size, shape, edge type, and electrostatic gating, e.g., see Refs. [4,5,10,16,20,33-35,39,42,43]. Interesting properties such as gap opening [11,33,43], appearing degenerate zero-energy edge states [4,10], and long-spin relaxation time [10], have been reported in these studies.

The electronic properties of untwisted AB- or AA-stacked BLG QDs have been studied both theoretically [11,16,38,41,42] and experimentally [15,17]. In a tBLG QD, twist angle can be used as a new knob to tune the electronic properties of the system. The energy levels and optical properties of small tBLG flakes were recently studied in Ref. [45] at zero magnetic field. In this study the obtained energy levels are highly influenced by the edge effects of the flakes. The electronic and transport properties of tBLG nanoribbons have also been investigated, in which the transport properties of the low-energy regime were determined by the interplay between the moiré pattern and the AB edges. Another study was devoted to the investigation of the electronic properties of tBLG flakes with irregular shapes. It was shown that the presence of one complete moiré spot in a tBLG flake is sufficient to reproduce the density of states of the corresponding tBLG sheet.

The purpose of this paper is to investigate the effect of twisting angle on the energy levels of circular tBLG QDs which are completely distinct structures from the AB- or AA-stacked BLG QDs (Fig. 2). To eliminate the effect of edges, we define a circular tBLG QD surrounded by a staggered site-dependent infinite-mass (IM) potential and experimentally induced by sandwiching the tBLG sheet between the top and bottom substrates such that the A and B sublattices in each graphene sheet feel a different potential.

Using the tight binding model (TBM), we obtain the energy spectra of tBLG QDs in both the absence and presence of an external magnetic field and demonstrate the effect of twisting on the energy levels. In Sec. II we briefly recapitulates the geometry of a tBLG lattice. The proposed QD structure in tBLG, and the basics of our numerical method are presented in Sec. III. In Secs. IV and V, we present our results for the energy levels and confined states in the absence and presence of a perpendicular magnetic field, respectively. A summary and concluding remarks follow in Sec. VI.
II. ATOMIC STRUCTURE OF TWISTED BILAYER GRAPHENE

In this section, we briefly review the atomic structure of tBLG. One can find more detailed and comprehensive study of the tBLG system in Refs.\textsuperscript{53-56}. Monolayer graphene (MLG) is a 2D honeycomb lattice of carbon atoms, whose unit cell contains two inequivalent sublattices, \( A \) and \( B \). Twisted BLG consists of two graphene layers which are twisted with respect to each other by an angle \( \theta \). We define the honeycomb lattice of graphene with the lattice vectors \( \mathbf{a}_1 = a(\sqrt{3}/2, 1/2) \) and \( \mathbf{a}_2 = a(\sqrt{3}/2, -1/2) \), where \( a \approx 0.246 \) nm is the lattice constant. In the lower layer (named layer 1), containing \( A1 \) and \( B1 \) sublattices, the lattice positions are given by

\[
\mathbf{r}_{A1} = m\mathbf{a}_1 + n\mathbf{a}_2,
\]

\[
\mathbf{r}_{B1} = m\mathbf{a}_1 + n\mathbf{a}_2 + \mathbf{\delta}_1,
\]

\[
(m, n) \in \mathbb{Z},
\]

where \( \mathbf{\delta}_1 = (\mathbf{a}_1 + \mathbf{a}_2)/3 \) connects the nearest-neighbor site inside the unit cell of the graphene lattice.

Here, we define the case of \( \theta = 0 \) as a perfect AA-stacked BLG, in which each carbon atom in the second layer (with \( A2 \) and \( B2 \) sublattices) is vertically displaced by \( d_0 = 0.335 \) nm (interlayer spacing) from the corresponding atoms in the first graphene sheet. In tBLG, the top graphene layer is rotated with respect to the lower layer by an angle \( \theta \) around a common site, e.g., \( A1-A2 \) position [Fig. 1(a)]. Accordingly, the primitive lattice vectors of the rotated layer are given by \( \mathbf{\tilde{a}}_i = \mathcal{R}(\theta)\mathbf{a}_i \) \((i = 1, 2)\), and, thus, its atom positions are

\[
\mathbf{r}_{A2} = m\mathbf{\tilde{a}}_1 + n\mathbf{\tilde{a}}_2 + d_0\mathbf{e}_z,
\]

\[
\mathbf{r}_{B2} = m\mathbf{\tilde{a}}_1 + n\mathbf{\tilde{a}}_2 + d_0\mathbf{e}_z + \mathbf{\tilde{\delta}}_1,
\]

where \( \mathcal{R}(\theta) \) is a \( 2 \times 2 \) rotation matrix, \( \mathbf{e}_z \) is the unit vector parallel to the \( z \) axis, and \( \mathbf{\tilde{\delta}}_1 = (\mathbf{\tilde{a}}_1 + \mathbf{\tilde{a}}_2)/3 \).

In general, the lattice structure of tBLG is not periodic for any \( \theta \) (incommensurate structure). However, in certain integers \( m \) and \( n \), it is possible that the lattice vector of layer 1, \( m\mathbf{a}_1 + n\mathbf{a}_2 \), coincides with the lattice vector of layer 2, \( m\mathbf{\tilde{a}}_1 + n\mathbf{\tilde{a}}_2 \), and the structure becomes periodic (commensurate structure). The superlattice structure is thus defined by the lattice vectors\textsuperscript{57}

\[
\mathbf{L}_1 = m\mathbf{a}_1 + n\mathbf{a}_2 = m\mathbf{\tilde{a}}_1 + n\mathbf{\tilde{a}}_2,
\]

\[
\mathbf{L}_2 = \mathcal{R}(\pi/3)\mathbf{L}_1.
\]

A commensurate twist angle with a periodic moiré pattern is given by

\[
\cos(\theta_{m,n}) = \frac{1}{2} \left( m^2 + n^2 + 4mn \right) - \frac{1}{2} \left( m^2 + n^2 + mn \right),
\]

and the lattice constant of the (commensurate) superlattice \( L_{m,n} = |\mathbf{L}_1| = |\mathbf{L}_2| \) is

\[
L_{m,n} = a\sqrt{m^2 + n^2 + mn} = \frac{|m - n|a}{2\sin(\theta/2)}.
\]

The label \((m, n)\) is used as a representative of a corresponding commensurate twist angle given by Eq. (4).

For twist angles \( \theta \lesssim 15^\circ \), due to the mismatch between the lattice vectors of the two layers, the moiré superlattice period \( L_M = a/2\sin(\theta/2) \) can be defined for any commensurate or incommensurate \( \theta \). Notice that \( L_{m,n} = |m - n|L_M \). Obviously, the lattice constant of commensurate superstructure \( L_{m,n} \) coincides with the moiré superlattice period \( L_M \) when \(|m - n| = 1\).

Figures 1(b) and 1(c) illustrate the atomic structure of tBLG when \( \theta_{6,7} = 5.09^\circ \) \((L_{6,7} = L_M, |m - n| = 1)\) and \( \theta_{6,8} = 9.43^\circ \) \((L_{6,8} = 2L_M, |m - n| = 2)\), respectively. The electronic properties of tBLG depend on these two length scales, \( L_{m,n} \) and \( L_M \).
edge boundaries in which the second MLG QD (top) is rotated by an angle $\theta$ around the geometry center of the dot. When $\theta = 0$, the system is a perfect AA-stacked BLG QD. The interlayer spacing is $d_0$.

We consider a circular tBLG dot region with radius $R$, surrounded by a site-dependent staggered potential with $M_0 = 2.0$ eV [Fig. 2(a)], such that the atoms belonging to the sublattices A1 (A2) and B1 (B2) have a mass-term potential of $+M_0$ ($-M_0$) and $-M_0$ ($+M_0$), respectively. The staggered potential eliminates the specific edge effects, e.g., appearance of the zero-mode states due to the zigzag edges.

We use a single-orbital TBM for $p_z$ atomic orbital of carbon, as introduced by Wallace\textsuperscript{60}. The TBM Hamiltonian in a second quantization formalism can be written as

\begin{equation}
H = \sum_i (\epsilon_i + M_i) c_i^\dagger c_i - \sum_{<i,j>} t(d_{ij}) c_i^\dagger c_j + \text{H.c.}, \tag{6}
\end{equation}

where $c_i^\dagger$ and $c_i$ are, respectively, the creation and annihilation operators for an electron on the lattice site $i$ with on-site energy $\epsilon_i$ and mass-term potential $M_i$. In the second term, $d_{ij} = R_i - R_j$ is the distance between the lattice points $(R_i, R_j)$, $t(d_{ij})$ is the corresponding transfer integral, and $<i, j>$ indicates a summation over nearest neighbor sites. In terms of the Slater-Koster form, the transfer integral between the atoms $i$ and $j$ can be written as\textsuperscript{55,61–65}:

\begin{align*}
-t(d_{ij}) &= V_{pp\sigma} \left[ 1 - \left(\frac{d_{ij} \cdot e_z}{d_{ij}}\right)^2 \right] + V_{pp\sigma} \left(\frac{d_{ij} \cdot e_z}{d_{ij}}\right)^2, \\
V_{pp\sigma} &= V_{pp\sigma}^0 \exp\left(-\frac{d_{ij} - a_{cc}}{\delta_0}\right)^2, \\
V_{pp\sigma}^0 &= V_{pp\sigma}^0 \exp\left(-\frac{d_{ij} - d_0}{\delta_0}\right)^2. \tag{7}
\end{align*}

where $a_{cc} = a/\sqrt{3} \approx 0.142$ nm is the carbon-carbon distance of graphene and $\delta_0 = 0.184a$ is the decay length. $V_{pp\sigma}^0 \approx -2.7$ eV and $V_{pp\sigma}^0 \approx 0.48$ eV are the intralayer and interlayer nearest-neighbor hopping parameters, respectively. For the interlayer coupling, we include only the nearest-neighbor hopping parameter. But for the interlayer coupling, since the layers are rotated and the neighbors are not on top of each other, we take the interlayer coupling terms for atomic distances of $d_{ij} \leq 4a_{cc}$\textsuperscript{55}. As a result of mixing between the two sublattices, the electron-hole ($e$-$h$) symmetry is broken.

In the presence of a magnetic field, the transfer energy becomes $t(d_{ij}) \rightarrow t(d_{ij}) e^{i2\pi\Phi_{ij}}$, where

\begin{equation}
\Phi_{ij} = \frac{1}{\Phi_0} \int_{R_i}^{R_j} A(r) \cdot dr, \tag{8}
\end{equation}

is the Peierls phase\textsuperscript{66} with $\Phi_0 = h/e$ the magnetic flux quantum and $A(r)$ the vector potential. The vector potential corresponding to the external magnetic field $B = B e_z$ perpendicular to the tBLG flakes is chosen in the Landau gauge $A = (0, Bx, 0)$ for which one finds that $\Phi_{ij}$ is only nonzero in the $y$-direction and is given by $\Phi_{ij} = \text{sgn}(y_j - y_i) \frac{(x_j - x_i)}{2\sqrt{3}a} \Phi$, where $\Phi = \sqrt{3}a^2 B/2$ is the magnetic flux threading one carbon hexagon ($a$ is the graphene lattice constant).

We also calculate the electron and hole current from site $j$ into site $i$ using\textsuperscript{50,51,67}

\begin{equation}
I_{ji} = \frac{2e}{h} \text{Im} \sum_{\gamma'\gamma} \mathcal{H}_{\gamma', \gamma} \phi_{\gamma'} \phi_{\gamma}^*, \tag{9}
\end{equation}

where $\mathcal{H}_{\gamma', \gamma}$ is the TB Hamiltonian matrix elements, $\{\phi_{\gamma}\}$ are the quantum states on the lattice sites, and $\gamma$ is the orbital index. The total current at each site $i$ can be obtained using

\begin{equation}
I_i = \sum_j I_{ji} \mathbf{f}_{ij}, \tag{10}
\end{equation}

where $\mathbf{f}_{ij}$ is the unit vector pointing from site $i$ to site $j$.

\section*{IV. ENERGY LEVELS: ZERO MAGNETIC FIELD}

In the absence of any external magnetic field, we first consider the energy spectrum of a circular tBLG QD as...
a function of the twist angle $\theta$ at a fixed radius $R$. Figure 3(a) shows the results for $R = 4.81$ nm. Due to the mass-potential confinement, the QDs exhibit an energy gap between the electron and hole states irrespective of the twist angle. For $10^\circ \lesssim \theta \lesssim 50^\circ$ the interlayer hoppings are weak, the two layers become effectively decoupled, and thus the energy levels are nearly independent of $\theta$ at this range. At $\theta = 0^\circ$ and $\theta = 60^\circ$, the tBLG structure turns into a prefect AA- and AB-stacked BLG QD, respectively (see the corresponding energy spectra in Refs.\textsuperscript{39,42}).

At $\theta \lesssim 10^\circ$ and $\theta \gtrsim 50^\circ$, the formation of moiré patterns with well-defined AA and AB-stacked spots (see Fig. 1), modifies the spectrum and a minimum energy gap appears at $\theta \approx 1.5^\circ$ and $\theta \approx 58.2^\circ$. Figure 3(b) shows the minimum energies of the first lowest-electron state (at $\theta < 10^\circ$) for different QD sizes (labels indicate the corresponding dot radius $R = 1.1$ nm $-$ 7.5 nm). We observe that the minimum energy occurs at smaller angles when the dot radius increases. When $R \approx L_{m,n}$ the minimum energy appears at $\theta < 1^\circ$ (see the red points in Fig. 3(b) for $R = 2.77$ nm $\approx L_{6.7}$ and $R = 3.62$ nm $\approx L_{8.9}$).

In order to better understand this, we define the spatial distribution of the probability densities corresponding to the $N$ lowest-electron-energy states as

$$\rho_{e,N} = \sum_{\ell,s} |\psi_{\ell,s}(\textbf{r})|^2,$$

where $\psi_{\ell,s}(\textbf{r}) = [\phi_{\ell,A}(\textbf{r}_s), \phi_{\ell,B}(\textbf{r}_{s'})]^T$ denotes the quantum state of the two layers ($\ell = 1, 2$) with energy $\epsilon_{\ell,s}$. The components $\phi_{\ell,A}(\textbf{r}_s)$ ($s = 1, 2, \cdots, N_{A\ell}$) and $\phi_{\ell,B}(\textbf{r}_{s'})$ ($s' = 1, 2, \cdots, N_{B\ell}$) correspond to the different sublattices $A\ell$ and $B\ell$ in each layer, respectively.

In Figs. 4(a)–4(e), we show $\rho_{e,N}$ for the four lowest-energy states ($N = 4$) shown in the spectrum of Fig. 3 at different twist angles (as labeled). In the case of $\theta = 0^\circ$ (AA-stacked BLG QD), the lowest-energy state is fourfold degenerate, (two for layer and two for valley degeneracy), for which the electrons are equally distributed in both layers [Fig. 4(a)]. As $\theta$ increases, the moiré lengths becomes smaller, and well-defined AA- and AB-stacked regions start to form in the QD area. At $\theta = 1.5^\circ$ (the angle at which the minimum energy of the lowest-electron energy occurs), the centrally confined AA-stacked region which is induced by the mass potential, hybridizes with the moiré-pattern-induced AA-stacked confined regions at the edge of the QD [Fig. 4(c)]. This decreases the energy gap slightly. As $\theta$ increases (moiré length decreases) the AA-stacked regions form inside the QD [Fig. 4(d)], a stronger hybridization occurs, and therefore the energy increases. We note that in a pristine tBLG sheet, the states near the Dirac points also localize in the AA-stacked spots of the moiré pattern\textsuperscript{62,68}. The semiclassical treatment of one-dimensional strained moiré in BLG\textsuperscript{69} shows that the energies near the Dirac point are trapped in a semiclassical potential centered at the AA spots and the electron localization is driven by this potential. Although the existence of such moiré potential wells in the AA regions of the tBLG structure has been discussed in Refs.\textsuperscript{51,68,70}, a systematic study (e.g., providing a semiclassical approach similar to the one in Ref.\textsuperscript{69}) is needed to rigorously show this existence. On the other hand, for large twist angles, the period of the commensurate structure is too small to create a well-defined AA- and AB-stacked regions and the system behaves as two decoupled monolayer [see Fig. 4(e) for $\theta = 32.20^\circ$]. We have observed similar patterns for different QD sizes (including a dot with only a single moiré spot, i.e., $R = L_{m,n}$).

Figure 5 shows the energy levels as a function of the dot radius $R$ for the five different twist angles (a) $\theta = 0^\circ$ (AA-stacked BLG QD), (b) $\theta = 1.08^\circ$ (magic angle), (c) $\theta = 5.09^\circ$, (d) $\theta = 32.20^\circ$, and (e) $\theta = 60^\circ$ (AB-stacked BLG QD). The low-energy levels exhibit a power-law decay as functions of $R$ and strongly depend on the twisting angle $\theta$. The red solid curves show power-law fits (up to $\epsilon \lesssim 0.17$ eV) to the lowest-electron energy level. The AA- and AB-stacked QDs [Figs. 5(a) and 5(e)], exhibit a $\sim 1/R$ and $\sim 1/R^2$\textsuperscript{11} dependence. These dependencies can be explained by the linear and quadratic low-energy dispersion in AA- and AB-stacked BLG sheets. A remarkable difference is seen at the magic twist angle $\theta = 1.08^\circ$ [Fig. 5(b)], for which the energy gap between the electron and hole states closes rapidly when the dot radius increases. The lowest electron energy in this case shows a $\sim 1/R^2$\textsuperscript{11} dependence. This behavior can be linked to the band flattening of the lowest moiré band at magic twist angles\textsuperscript{53,54,71}. At $\theta = 32.20^\circ$ we found that the interlayer coupling becomes extremely weak, the two layers are decoupled, and therefore the corresponding spectrum in Fig. 5(d) exhibits two copies of a monolayer graphene QD spectrum. This statement can also be confirmed through the localization of the charge density.
FIG. 4. Probability densities corresponding to the four lowest-electron-energy levels shown in the energy spectrum of Fig. 3 with $R = 4.81$ nm. The results are presented for five different twisting angles (a) $\theta = 0^\circ$ (AA stacking), (b) $\theta = 1.08^\circ$ (magic angle), (c) $\theta = 1.53^\circ$, (d) $\theta_{6,7} = 5.09^\circ$, and (e) $\theta_{1,3} = 32.20^\circ$. Layer 1 (2) is represented by the blue (red) color and the yellow region indicates the mass potential barrier.

shown in Fig. 4(e) for $\theta_{1,3} = 32.20^\circ$. Our fittings for the twisting angles $\theta_{6,7} = 5.09^\circ$ and $\theta_{1,3} = 32.20^\circ$ show a $\sim 1/R$ dependence.

V. LANDAU LEVELS

Here, we investigate the effect of a perpendicular magnetic field on the energy levels of tBLG QDs. As pointed out in Sec. IV, at large twist angles, a tBLG QD behaves as two decoupled monolayer QDs. Accordingly, we present our results for the small twist angle $\theta_{6,7} = 5.09^\circ$ and compare with the case of an untwisted AA-stacked BLG QD ($\theta = 0$).

Figure 6 shows the magnetic levels, i.e., the so-called Fock-Darwin levels, of a circular tBLG QD with $R = 4.81$ nm, as functions of the magnetic flux threading one carbon hexagon $\Phi$ (in the units of $\Phi_0$) for (a) $\theta = 0$ (untwisted) and (b) $\theta_{6,7} = 5.09^\circ$. The Landau levels (LLs) in an AA-stacked BLG QD [$\theta = 0$, Fig. 6(a)], exhibit a band gap between the electron and hole levels for the whole range of magnetic field. As magnetic field increases, the discrete low-energy levels approach asymptotically the LLs of an AA-stacked BLG sheet for which the zeroth electron (hole) LLs are $\epsilon_A^{(0)} = \gamma_+ \approx +0.37$ eV where $\gamma_+$ is the average interlayer coupling between the neighboring atoms (with cutoff $4\pi a_c^2$). Figure 6(b) shows the LLs of a tBLG QD with the twist angle $\theta_{6,7} = 5.09^\circ$. A small twisting significantly affects the magnetic levels in tBLG QDs. As $B$ increases, the energy gap closes and the lowest magnetic levels spread out between the electron and hole zeroth LLs of a pristine tBLG, which are different than those of AA- or AB-stacked BLG. These are edge states, localized at the boundaries between the AA- and AB-stacked regions. Figure 6(c) shows the corresponding density distribution $\rho_{N1}$ at $\Phi = 0.02\Phi_0$ ($l_B = \sqrt{\hbar/eB} = 0.66$ nm $< L_{6,7} = 2.77$ nm), where we summed over the energies with $|\epsilon_{N1}| \leq 0.15$ eV. For the energy range of $0.15$ eV $< |\epsilon_{N2}| \leq 0.24$ eV, farther from $\epsilon_F$, one can see that the carrier is mostly localized at the AA spots of the moiré pattern, Fig. 6(d). Approaching the tBLG LLs, as a result of coupling between the moiré-lattice- and the magnetic-field-induced states, anticrossings appear in the spectrum.
Note that, at the low magnetic fields, for which the magnetic length $l_B$ is greater than the moiré length $L_{m,n}$, the results (not shown here) are very similar to the case $B = 0$ (Sec. IV). We also note that, since we have considered small sizes of the dots, the applied magnetic field in our calculations are too high to be achievable in experiments. However, in QDs, one can define a scaling factor and thus extend the results to lower $B$ and larger QD sizes\textsuperscript{74}. By setting the dot size $R$ equal to the cyclotron radius at the Fermi energy, i.e., $R = l_B^2 k_F$ and using $E \approx \pm V_0^\sigma \pm \hbar v_F k_F$ for the low-energy dispersion of the AA-stacked BLG, one can obtain $k_F$ and consequently the scaling factor with respect to the magnetic field and size of the confinement area as $R = (E \pm V_0^\sigma)/(\hbar v_F B)$. For the typical values of $E = \pm V_0^\sigma = 1$ eV, $v_F = 10^6$ m/s, and $B = 20$ T, we obtain $R = 50$ nm.

Finally, we consider the electron current of tBLG QD using Eqs. (9) and (10). The in-plane (interlayer) current at site $i$ is defined as the sum of all outgoing current vectors from site $i$ to other sites (to all sites in the other layer)\textsuperscript{51}. In Fig. 7, we plot the current densities for a dot of radius $R = 4.81$ nm and the twist angle of $\theta_{6,7} = 5.09^\circ$ ($L_{6,7} = 2.77$ nm). The results are shown for two different magnetic fields (upper panel) $\Phi = 0.005 \Phi_0 \ [B = 40 \ T, l_B = 4.06 \text{nm} > L_{6,7}]$ and (lower panel) $\Phi = 0.0025 \Phi_0 \ [B = 200 \ T, l_B = 1.81 \text{nm} < L_{6,7}]$. Panels (a,d) and (b,e), respectively, show the in-plane current vectors in layers 1 and 2, summed over the first two electron states shown in the energy spectrum of Fig. 6(b). Corresponding interlayer currents are displayed in panels (c) and (f). As seen, irrespective of the ratio between $l_B$ and $L_{m,n}$, the current densities are affected by the moiré pattern. In both cases, the interlayer current flows from layer 1 into layer 2 through the AA spots (light regions) and back through the AB spots (dark-blue regions). The similar effect was observed for other tBLG nanostructures\textsuperscript{50,51}. As can be seen in Figs. 7(a,b), when $l_B > L_{m,n}$, the in-plane current components, with anticlockwise motion in both layers, flow toward the centeral AA spot in layer 1, and outward in layer 2. The centeral AA and its neighboring AB spots have the highest interlayer current density [Fig. 7(c)] and the lowest in-plane current density [Fig. 7(a,b)]. At a high magnetic field ($l_B < L_{m,n}$), one can obviously observe the increase of the interlayer current [cf. Figs. 7(c) and 7(f)]. On the other hand, the in-plane current components in each layer flow in opposite directions between the adjacent source and sink regions of the interlayer current, see Figs. 7(d) and 7(e).

VI. SUMMARY AND CONCLUDING REMARKS

In summary, using a tight binding model we studied the electronic properties of circular QDs in twisted bilayer graphene defined by infinite-mass boundary conditions, and investigated the effect of twisting angle on the energy levels and the corresponding density distributions in the absence and presence of a perpendicular magnetic field $B$. In the absence of magnetic field, or when the magnetic length is greater than the moiré length ($l_B > L_{m,n}$), the low-energy levels are affected by the formation of moiré pattern where the carriers confine at the AA-stacked regions. We found that, due to the hybridization between the mass-induced confinement and the AA-stacked localized states, the energy spectrum...
FIG. 7. Electron current density profile for a tBLG QD of radius $R = 4.81$ nm and with the twist angle of $\theta_{6,7} = 5.09^\circ$ ($L_{6,7} = 2.77$ nm). Upper (Lower) panel shows the result for $B = 40$ T ($B = 200$ T) for which $l_B > 4.06$ nm > $L_{6,7}$ ($l_B = 1.81$ nm < $L_{6,7}$). Panels (a,d) and (b,e), respectively, show the in-plane current vectors in layers 1 and 2, corresponding to the first two electron states shown in the energy spectrum of Fig. 6(b). (c,f) Corresponding perpendicular interlayer current flowing between the dot layers. Light and dark regions, respectively, indicate the current directions out and into of the dot plane.

changes for small twist angels $\theta \lesssim 10^\circ$. In the presence of a strong magnetic field where $l_B < L_{m,n}$, the energy gap of the untwisted QDs ($\theta = 0$) closes and the lowest LLs spread out over the gap, and are associated with the edge states localized at the boundaries between the AA- and AB-stacked regions.

Electron current investigation also showed that, irrespective of the ratio between the magnetic and moiré lengths, applied perpendicular magnetic field causes interlayer charge flow between the dot layers, forming source and sink regions of the interlayer current at the AA and AB spots over the dot region. On the other hand, the in-plane current density profile exhibits different pattern depending on the ratio between the magnetic and moiré length scales.

ACKNOWLEDGEMENTS

We gratefully acknowledge discussions with I. Snyman.

* mohamad.mirzakhani@gmail.com
† francois.peeters@uantwerpen.be
‡ zareniam@missouri.edu