Electronic conductance of twisted bilayer nanoribbon flakes

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We study the transport properties of a twisted bilayer graphene flake contacted by two monolayer nanoribbons. We analyze the conductance in terms of the spectra of the bilayer nanoribbon and the leads. Depending on the number of available conduction channels in the flake, transport resonances and antiresonances in the system can be identified. The low-energy transport properties are governed by the edge states with AB stacking. In contrast with the conductance of bilayer flakes with more symmetric stackings, their characteristics in this energy region do not depend much on the relative position of the leads, but are related to the AB edge regions of the flake.

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I. INTRODUCTION

The electronic properties of graphene can be tuned by stacking a few layers of this material [1, 2]. This opens a way to tailor its band structure and even open a gap by the application of an electric field [3–6]. In fact, the low-energy band structure of bilayer graphene strongly depends on the stacking sequence. While AA stacking preserves the linear dispersion around the Fermi level, typical for a single layer [7, 8], AB-stacked graphene has a parabolic dispersion relation [9–11]. Furthermore, rotating the two layers is yet another way to modify the spectrum of bilayer graphene that has been also explored [12–18]. In this latter system, also called twisted bilayer graphene (TBG), the rotation angle between layers determines the electronic properties of the system and different electronic regimes have been identified [19, 20]. For large rotation angles, the system behaves as two noninteracting monolayers, while for small rotation angles, below 10°, the Fermi velocity decreases, dropping to zero around the angle of 1°[21, 22]. Moreover, scanning tunneling measurements have revealed large superperiodicities in the density of states of TBG, described as moiré patterns [13]. Regions with different types of stacking, AA and AB, as well as displaced graphene layers, called slip regions, can be identified. These areas have distinct electronic localizations depending on the energy, giving rise to inhomogeneous distributions of the electrons.

Besides the opening of a gap, the application of graphene in nanoelectronics requires the realization of nanometric-size structures for the design of devices. Graphene nanoribbons emerge as optimal candidates for the development of carbon-based components at the nanoscale, with the added possibility of modifying its electronic properties because of finite-size effects [23–26]. Indeed, the electronic properties of monolayer nanoribbons strongly depend on their width and edge shape [27–31]. In the case of bilayer ribbons, the role of stacking has to be considered additionally [32–35]. In particular, for zigzag nanoribbons with AA stacking, the edge flat bands at the Fermi level split, while for AB-stacked zigzag nanoribbons, the edge bands are degenerate at the Fermi level. This difference can be explained in terms of the larger interlayer coupling in AA stacking, which splits the edge bands in bonding and antibonding.

The electronic transport properties of bilayer graphene flakes have also been recently addressed for the most symmetric geometries, i.e., zigzag and armchair edges and direct (AA) and Bernal (AB) stackings [36–39]. An oscillating behavior of the conductance with respect to the energy, flake length and interlayer coupling was reported. Such transport characteristics are relevant for the design of electromechanical devices, and deserve further exploration in more general geometries, such as moiré bilayer ribbons and chiral edges.

In this work we study the transport properties of twisted bilayer graphene nanoribbons. By cutting a stripe from a twisted bilayer graphene, different atomic stackings may appear at the edges. Therefore, an interplay between the moiré pattern and the graphene edges is expected to govern the low-energy transport through these systems [40]. Although there is no controllable way to fabricate them, twisted bilayer structures appear naturally in some growth methods [16, 18]. Moreover, unzipping multiwall nanotubes can be used to obtain twisted bilayer nanoribbons [41, 42].

In order to investigate the electronic transport properties of twisted bilayer nanoribbons, we consider a bi-
layer flake connected to monolayer leads, as previously done for armchair and zigzag bilayer ribbons with AA and AB stackings [36, 37]. We analyze the appearance of localized states near the Fermi energy, and explore their origin, i.e., their relation to edge and bilayer stacking, as well as their role in the conductance of the system.

II. GEOMETRY

In this Section we briefly describe the geometry of the system studied, a bilayer graphene ribbon with monolayer ribbon contacts.

A. Twisted bilayer nanoribbon

We build the unit cell (UC) of the twisted bilayer nanoribbon in the same way as in Ref. 40 (see Fig. 1), from that of twisted bilayer graphene. Recall that the UC for commensurate twisted bilayer is generated by rotating one of the AB-stacked layers about an axis passing through a B atom, so that an atom with coordinates \( \vec{r} = m\vec{a}_1 + n\vec{a}_2 \) is rotated to an equivalent site \( \vec{t}_1 = n\vec{a} + m\vec{a}_2 \). Here \( \vec{a}_1 = \frac{2}{\sqrt{3}}(\sqrt{3}, -1) \) and \( \vec{a}_2 = \frac{2}{\sqrt{2}}(\sqrt{3}, 1) \) are the graphene lattice vectors and \( a = 2.46 \, \text{Å} \) is the graphene lattice constant. The relative rotation angle (RRA) is completely specified by the integers \( n \) and \( m \), namely, \( \cos \theta = (n^2 + 4nm + m^2)/(2(n^2 + nm + m^2)) \). The unit cell of the system is defined by the vectors \( \vec{t}_1 = n\vec{a} + m\vec{a}_2 \) and \( \vec{t}_2 = -m\vec{a}_1 + (n + m)\vec{a}_2 \), which span an angle of 60°. Since the two integers \( n \) and \( m \) fully determine the unit cell, they are usually chosen as labels for the moiré bilayer, \( (n, m) \). We select them to fulfill the condition of \( n = m + 1 \). In principle, a twisted bilayer nanoribbon can be generated by repeating the UC along the directions given by \( \vec{t}_1 \) or \( \vec{t}_2 \), but this would produce edges with a dominant armchair component. As zigzag-terminated edges have low-energy, edge-localized states, with remarkable transport properties, we choose another unit cell, with a translation vector \( \vec{T} = 2\vec{t}_2 - \vec{t}_1 \) perpendicular to \( \vec{t}_1 \), so that the edge runs along \( \vec{T} \). This rectangular UC is twice the size of the minimal one, but with an edge vector \( \vec{T} = (2m+n, n-m) \) with mostly zigzag character. For \( n = m + 1 \) this implies that \( \vec{T} = (3m+1, 1) \). We choose the edges to be minimal, i.e., with a minimum number of edge atoms with coordination number 2 [28, 30]. Following Ref. 40, twisted bilayer nanoribbons are labeled indicating the coordinates of the edge vector \( (3m+1, 1) \) and the moiré pattern in brackets \( [(n,m)] \), that is, \( (3m+1, 1)/[(n,m)] \). Although this information is redundant, it helps to identify more easily the geometry of the ribbons. We omit in this work the width index because all examples chosen herein have the same, equal to \( |\vec{t}_1| \), so it would be always equal to 1 in units of the bilayer nanoribbon width vector \( \vec{t}_1 \).

B. Bilayer flake with monolayer leads

We construct the flake by connecting the finite twisted bilayer ribbon with semiinfinite monolayer leads with the same edge vectors and widths. As previously done with achiral ribbons [36], we consider two ways of devising a finite-size bilayer flake with contacts. First, we put a flake on top of an infinite ribbon (Fig. 2 (a)), so that the monolayer parts of the system play the role of leads. We refer to this as the 1-1 or island configuration.

Second, the leads are connected to different layers of the flake, so the system can be viewed as two overlapping semiinfinite ribbons (Fig. 2 (b)). We will refer to it as the 1-2 or overlap configuration. As our interest is to elucidate the interplay of edge states and the moiré pattern, which produces different stackings on the edge, we avoid other sources of localization by choosing all edges to be...
minimal in both configurations, without Klein atoms [43], coves or capes, and having an armchair shape at the ends of the flake.

III. MODEL AND METHOD

We model the system with a $p_z$-orbital tight-binding Hamiltonian. For the monolayer ribbons constituting the leads we consider only the nearest-neighbor hopping parameter $\gamma_0 = -3.16$ eV and on-site energy $\epsilon_0 = 0$.

For the bilayer flake, the Hamiltonian can be written as

$$H = H_1 + H_2 + H_{12},$$

where $H_1$ and $H_2$ are single-layer Hamiltonians and the interlayer Hamiltonian $H_{12}$ is given by

$$H_{12} = \sum_{i,j} \gamma_1 e^{-\beta(r_{ij}-d)} c_i^\dagger c_j + H.c.,$$

where $\gamma_1 = -0.39$ eV is the interlayer hopping, $r_{ij}$ is the distance between in-plane coordinates of atoms $i$ and $j$ belonging to different layers, $d = 3.35$ Å is the distance between layers, and $\beta = 3$ is a parameter fitted to the density functional theory calculations [14, 15]. We take a cutoff for the interlayer interaction of $6a_{CC}$, with $a_{CC} = 1.42$ Å.

Since the bilayer flake with leads has no translation symmetry, we use the Green function matching method to compute the density of states and the conductance. The total Hamiltonian of the system is given by [44]:

$$H = H_L + H_R + H_C + V_{LC} + V_{RC},$$

where $H_L$ and $H_R$ are the Hamiltonians of the left (L) and right (R) lead respectively, single-layer ribbons in this case, $H_C$ is the Hamiltonian of the central part or conductor, i.e., the twisted bilayer flake, and $V_{LC}$ and $V_{RC}$ are the connections of the conductor to the left and right lead, respectively. The Green function of the conductor $C$, which a function of the energy $E$, is then [44]

$$G_C(E) = (E - H_C - \Sigma_L - \Sigma_R)^{-1}$$

where $\Sigma_L = V_{LC} g_L V_{LC}^\dagger$ and $\Sigma_R = V_{RC} g_R V_{RC}^\dagger$ are the leads self-energies and $g_{L,R}$ are the Green functions of the monolayer leads.

The conductance is calculated using the Landauer-Büttiker formalism,

$$G = \frac{2e^2}{h} T(E) = \frac{2e^2}{h} Tr[\Gamma_L G_C \Gamma_R G_C],$$

where $T(E)$ is the transmission function from the left lead to the right one and $\Gamma_{L,R} = i[\Sigma_{L,R} - \Sigma_{L,R}^\dagger]$ describe the coupling between the conductor and the $L, R$ leads.

IV. RESULTS AND DISCUSSION

Most of our results will be shown for $(10,1) [(4,3)]$ bilayer flakes, with RRA equal to $\theta = 9.43^\circ$. We have also performed calculations for smaller systems, like $(4,1)[(2,1)],$ and larger systems, such as $(13,1)[(5,4)]$. However, on the one hand, for ribbons with smaller unit cells and large RRA, the moiré pattern is too small to observe a clear AA and AB edge stacking. On the other hand, when the flake unit cell is very large, the analysis becomes too cumbersome, because the spectrum is much denser with numerous quasi-localized states very close in energy. The selected system, $(10,1)[(4,3)]$, is large enough to distinguish AA and AB stacking at the edges, and has a clearer spectrum, having all the relevant characteristics of larger ribbons.

Unless stated otherwise, the length of the flake is equal to two unit cells of the twisted bilayer ribbon. Thus we may distinguish stacking-related localization from that due to the finite-size of the flake.

Before carrying on with the results for the flakes, it is worthy to summarize previous research on the electronic properties of the constituent media, namely, the monolayer ribbons, which play the role of contacts, and the twisted bilayer nanoribbon constituting the conductor. In Fig. 3 we plot the band structures of the corresponding infinite ribbons: (a) the monolayer chiral ribbon with edge vector $\tilde{T} = (10, 1)$, and (b) the $(10, 1)[(4, 3)]$ twisted bilayer ribbon. The $(10,1)$ edge has 2 edge states [39], so the monolayer ribbon has 4 edge bands close to the Fermi energy, roughly between $-0.15$ eV and $0.15$ eV. As the ribbon is narrow, edge-localized states couple, so the edge bands have a relatively large dispersion that decreases for wider ribbons.

For the twisted bilayer nanoribbon we thus expect 8 edge bands, that we observe from $-0.25$ to $0.25$ eV. In this case, there is a difference between localization depending on the stacking. States closer to the Fermi level are mostly localized on the AB-stacked regions of the edges, while edge states farther from Fermi energy, around $|E| \approx 0.2$ eV, localize on regions with AA stacking [40]. Such energy difference related to the type of stacking can be clearly understood considering edge states in bilayer zigzag ribbons [40]. As mentioned before, edge states for AB-stacked ribbons are degenerate at $E_F$, whereas AA stacking splits the edge bands away from $E_F$ an amount related to the interlayer coupling. In twisted bilayer ribbons, edges have a mixture of different stackings; nonetheless we can verify that such relation between stacking and edge bands splitting remains.

A. LDOS and conductance of bilayer flakes

First we consider the 1-1 configuration, a monolayer nanoribbon with a finite-size graphene flake on top. Fig. 4 depicts the local density of states in the flake along with the conductance through this system. The right-
most panel (c) represents the conductance of the infinite bilayer flake, which allows us to have in mind the number of conductance channels in the conductor as well the available lead states: pink rectangles mark the energy gaps in the infinite single layer ribbon (10,1), which otherwise has one conductance channel in the depicted energy range. The conductance of the infinite systems is computed just by counting states.

We can easily correlate the peaks in the LDOS (Fig. 4 (a)) with distinct features in the conductance through the flake (Fig. 4 (b)). Notice that they have a remarkable energy dependence. In the region closer to $E_F$, energies $|E| < 0.15$ eV, they correspond to conductance maxima, and from the bulk band structure presented in Fig. 3, we infer that they correspond to AB-localized edge states in the flake. Likewise, we expect some maxima in LDOS and conductance around $|E| \approx 0.2$ eV to be caused by AA-localized edge states. For energies farther from $E_F$ the situation is more complex. If there are two available states in the conductor, antiresonances take place [45]. As depicted in panel (c), the two-channel energy ranges happen for $|E| \gtrsim 0.3$ eV, plus three narrow spikes due to a slight band bending of edge bands. The antiresonance behavior is clearly seen at $-0.29$ eV, where the LDOS peak matches a clear conductance zero minimum. In these cases, there is a destructive interference between the two available states in the conductor. The two LDOS peaks at $E = 0.42$ eV and $E = -0.43$ eV are two clear examples of this antiresonant behavior. This behavior was also observed in graphene flakes with more symmetric stackings [36].

The conductance of the island flake, Fig. 4 (b), presents clear gaps that correspond to those in the monolayer leads, marked as pink bands in panel (c). Notice, however, that there is a non-negligible conductance in energy windows without available states in the bulk bilayer conductor, such as from $0.1$ to $0.2$ eV or from $-0.2$ to $-0.06$ eV (see panel (c)). In these regions there are broad conductance peaks and shoulders due to tunneling through the flake. This is related to the small size of the central conductor, which is $50$ Å, but only two unit cells long.

The results for the 1-2 configuration, two overlapping semiinfinite nanoribbons producing a bilayer flake, are shown in Fig. 5. Although the quantitative values differ, the analysis is similar: LDOS peaks around $E_F$ correspond to quasi-localized states that give rise to conductance maxima, due to the presence of only one available state in the flake. For $|E| \gtrsim 0.3$ eV, there are two available states in the flakes, so quasi-localized states produce an destructive interference giving rise to a conductance antiresonance.

Therefore, in both geometries, for the energy ranges for which the bilayer flake has only one available state, LDOS peaks correspond to conductance maxima. In such cases, the presence of quasi-localized states increases the probability of transmission through the flake. On the contrary, when there are two possible paths through the conductor—also signaled by a LDOS peak which indicates the presence of quasi-localized states—a zero conductance minimum reveals the interference between those two conduction channels.

**B. Spatial localization of flake states**

It is interesting to check the spatial localization of the states which give rise to the main conductance features, in order to verify our analysis based on the energy dependence of the AA- and AB-stacked edge states. As the size of the chosen system is still manageable, we have examined all the quasi-localized states in the energy range $[-0.5, 0.5]$ eV. Three different examples of localization can be seen in Fig. 6, for the case of the island flake, the 1-1 configuration. On the one hand, panel (a) presents a clear example of AB-edge localized state, with an energy $E = -0.0186$ eV. This energy value also confirms its AB-edge state origin. On the other hand, panel (b) is an instance of AA-localized flake state, with $E = -0.0221$ eV, which also matches the energy range of the AA-edge bands in the twisted bilayer ribbons. For energies $|E| > 0.3$ eV we observe the states related to the finite size of the flake, and indeed they are spread all over the flake region (Fig. 6 (c)).

The differences between the spatial distribution of the states can be related to those in the infinite twisted bilayer nanoribbon. For both configurations, states with energies close to the Fermi level ($|E| < 0.15$ eV) are mostly localized on the AB-stacked part of the edges,
whereas states that are slightly farther from \( E_F \) (|\( E \)| around 0.2 eV), have an LDOS concentrated on the AA-stacked edges.

When the energy \(|E| < 0.3 \text{ eV}\), a similar behavior is observed for the overlap flake. Fig. 7 (a) is an AB-edge state, rather similar to the corresponding case in the island flake, and also with an energy very close to \( E_F \), \( E = -0.0195 \text{ eV} \), belonging to the AB bands of the infinite bilayer nanoribbon. The same happens to the AA-localized state with energy \( E = -0.2213 \text{ eV} \), Fig. 7 (b): in these two cases, confinement is due to the interplay of the moiré pattern and the edges, not to the boundaries of the flake, where in fact the LDOS is almost negligible. This explains the similarities in these edge-localized flake states for the two configurations. However, the different boundary conditions for the bilayer flake result in distinct behaviors in the overlap and the island flake in energies \(|E| > 0.3 \text{ eV}\). LDOS maxima of these states correspond mainly to flake states, from quantum size effects for the whole system, not particularly localized at the edges. Fig. 7 (c) represents the LDOS for the \( E = 0.5025 \text{ eV} \), which corresponds to an antiresonance in the conductance. Here the quasi-localized state is spread all over the flake region. For energies \(|E| > 0.3 \text{ eV} \), the peaks correspond to Fabry-Perot states in the overlap system (Fig. 7 (c)), or quantum dot in the island case, (Fig. 6 (c)), for which localization in the upper flake is stronger. Contrary to the AB and AA-stacked edge localized states, these are only due to the boundary conditions of the flake, i.e., size effects. This different type of confinement explains the distinct behavior of the conductance for energies closer to \( E_F \) compared to energies corresponding to flake states, observed in Figs. 4 and 5.

Although AB-stacked edge states always lie close to \( E_F \), and AA-edge localized states are also roughly split an energy related to the interlayer coupling \(|\gamma_1|\), the rest of energy ranges mentioned above depend on the width of the flake and also of the RRA. For wider ribbons the dispersion of edge states is smaller, and the bulk bilayer nanoribbon bands shift closer to the Fermi energy, so the related flake antiresonances will also occur at smaller energies. Smaller RRA imply more edge states for the chiralities chosen in this work, but their behavior will be the same as reported for the (10,1) [(4,3)] flake.

Notice that, even though the antiresonances reported here correspond to flake states, not to those mainly edge-localized, for longer ribbons edge-localized states may also give rise to conductance minima. As discussed before, there are a few narrow two-channel energy windows corresponding to edge bands in which antiresonances may appear for sufficiently large flakes. In spite of these quantitative differences, the overall behavior described here can be easily extrapolated to other geometries.
FIG. 6. (Color online). LDOS for three states of 1-1 configuration exemplifying different types of localized states. (a) AB-stacking edge state at $E = -0.0186$ eV; (b) AA-stacked edge state at $E = -0.2210$ eV; and (c) flake state at $E = -0.4320$ eV. The radii of the circles are proportional to the LDOS value on each node. Color indicates localization on the bottom (red) and top (blue) layer.

FIG. 7. (Color online). LDOS for three states of an overlap flake with different localizations. (a) $E = -0.0195$ eV, edge state with AB stacking; (b) $E = -0.2213$ eV, edge state with AA stacking; and (c) $E = 0.5025$ eV, flake state. The radii of the circles are proportional to the LDOS value on each node. In panel (c) LDOS values are multiplied by 20. Color indicates localization on the bottom (red) and top (blue) layer.

C. Length dependence

We have also studied the dependence of conductance on the flake length. The results for both configurations are shown on Fig. 8. We select three energy values with distinct transport properties. In the first case, $E = -0.35$ eV, the bilayer flake has two propagating channels. Large-period oscillations can be observed with abrupt antiresonances, characteristic of the two-channel interference. Not all the conductance drops reach zero value due to the discrete sampling of the flake length, $N$ being an integer. For the second case, $E = -0.25$ eV, we observe an exponential decay of the conductance. This corresponds to a gap in the bilayer flake spectrum: for small $N$, there is a non-zero conductance due to tunneling, but for larger flakes transmission cannot occur through the bilayer, which acts as a barrier. In the third case, $E = -0.20$ eV, there is a clear oscillatory behavior. However, there are not antiresonances due to the existence of only one transmission channel in the flake, so the conductance does not drop below $C_{\text{min}} = 0.3 \frac{2e^2}{h}$. Obviously, this $C_{\text{min}}$ is different for other energy values, like in the symmetric flakes [36]. Notice that for $E = -0.35$ eV the conductance in island and overlap configurations has a complementary behavior. Such complementarity was also observed in armchair flakes with AA and AB stackings, most noticeably in the region with two propagating channels [36]. In chiral moiré flakes it can be also seen for energies $|E| > 0.3$ eV, for which two interfering channels exist. The other two cases presented in Fig. 8 are examples of tunneling through the flake ($E = -0.25$ eV), with exponentially decaying LDOS through the bilayer flake, and of AA-stacked edge state ($E = -0.20$ eV), for which the maximum weight of the LDOS is away from the leads-flake connections. Therefore, these two latter cases do not depend strongly on the particular lead configuration.
V. SUMMARY

We have studied the transport properties of twisted bilayer flakes connected to monolayer leads in two geometries, the island configuration, i.e., a monolayer ribbon with a finite-size flake on top, and the overlap configuration, composed of two overlapping monolayer ribbons which yield a twisted bilayer flake. These bilayer flakes are built forming a moiré pattern, so different stackings take place at the edges. The conductance through the flake shows resonant transport, tunneling and antiresonances depending on the number of available channels at the bilayer flake. We explain these different features by analyzing the energy spectra of the leads and the bilayer nanoribbon composing the system. Localized states related to the edges show a transport behavior which does not depend much on the configuration of the leads. For the case described in detail here, the (10,1) [(4,3)] bilayer flakes, this behavior corresponds to energies $|E| < 0.3$ eV. In general, the low-energy transport properties are governed by the AB-stacked edge states. Further away from the Fermi level, we observe states localized on the AA-stacked regions of the edges. For energies $|E| > 0.3$ eV, we observe localized states spread over the whole flake. Such states show a strong dependence on the configuration of the leads. In general, the interplay of moiré and edge states are responsible for the transport properties around the Fermi energy, which are qualitatively different to those of achiral flakes with symmetric stackings.

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