Electronic properties of a biased graphene bilayer

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We study, within the tight-binding approximation, the electronic properties of a graphene bilayer in the presence of an external electric field applied perpendicular to the system—biased bilayer. The resultant finite bias voltage between graphene planes gives rise to a finite gap in the spectrum, whose size is completely controlled by the applied voltage. The effect of the perpendicular electric field is included through a parallel plate capacitor model, with screening correction at the Hartree level. The model is applied to real biased bilayer devices, either made out of SiC or exfoliated graphene, and good agreement with experimental results is found, indicating that the model is capturing the key ingredients, and that a finite gap is effectively being controlled externally. Analysis of recent experimental results regarding the electrical noise and cyclotron resonance further suggests that the model can be seen as a good starting point to understand the electronic properties of graphene bilayer. The full tight-binding description is compared with its 4-band and 2-band continuum approximations, and the 4-band model is shown to be always a suitable approximation for the conditions realized in experiments. Also, we study the effect of electron-hole asymmetry terms, as the second-nearest-neighbor hopping energies $t'$ (in-plane) and $\gamma_4$ (inter-layer), and the on-site energy $\Delta$. Finally, we also study the electronic spectrum of the problem in the presence of a perpendicular magnetic field and discuss the nature of the quantum Hall effect in this system.

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I. INTRODUCTION

In his studies of the graphite band structure, Wallace¹ found that a single graphite plane (that is, graphene) has a linearly dispersing electronic spectrum at the corners of the hexagonal Brillouin zone (BZ) given by:

$$|E - E_c| \simeq \frac{\sqrt{3}}{2} \gamma_0 |k - k_c|,$$  \hspace{1cm} (1)

where $E_c$ is the on-site carbon energy, $\gamma_0$ is the nearest-neighbor (NN) hopping energy ($\gamma_0 = t$ in what follows), $a$ is the size of the unit cell vectors, and $k_c$ is the momentum at the hexagonal BZ corners (the $K$ and $K'$ points). This dispersion relation is the same as for massless relativistic Dirac fermions with an effective speed of light $v_F = \frac{te}{\hbar} = \frac{\sqrt{3}}{2}$. The recent discovery of graphene² the first truly one-atom thick material enabled several previously unthoughtful experiments where charge carriers were undoubtedly shown to be massless with a linear dispersion relation $\pm \sqrt{p^2 + \frac{\hbar^2}{m^2}}$, providing evidence for the massless excitations predicted by Wallace.

In addition to graphene, few-layer graphene can also be isolated. Of particular interest to us is the double layer graphene system, where two carbon layers are placed on top of each other according to the usual Bernal $AB$-stacking. The low-energy properties of this so-called bilayer graphene (BLG) are then described by massive Dirac fermions,⁷ with a quadratic dispersion close to the neutrality point and a Dirac fermion mass originating from the inter-plane hopping energy $t_\perp$.

The measurement of an anomalous integer quantum Hall effect (QHE) in single layer graphene (SLG)¹¹,¹² followed by the measurement of an integer QHE in BLG, characterized by the absence of a plateau at the Dirac point, were probably two of the most expressive experimental results of the last few years in condensed matter physics. Whereas the anomalous integer QHE in SLG is attributed to the massless Dirac fermions,¹¹,¹² which present a zero energy mode (leading to a zero energy Landau level in the presence of a magnetic field), the anomalous integer QHE in a BLG is associated with massive Dirac fermions and two zero energy modes.

The abovementioned findings make graphene and its bilayer very appealing not only from the point of view of fundamental physics but also from the point of view of applications. High mobilities even at high charge carrier concentrations, which seem to be little affected by chemical doping, have been recently reported in graphene.¹⁶,¹⁷,¹⁸,¹⁹ Indeed, intrinsic mobilities in both SLG and BLG exceed known values for any other semiconductor even at room temperature.²⁰,²¹,²² Furthermore, ballistic transport on submicron distances has also been observed,²³,²⁴ making graphene-based materials promising candidates for electronic devices.

The double-layer graphene is now a subject of considerable interest due to its unusual properties.²⁵,²⁶,²⁷,²⁸ Dissimilar in large extent to those of the single layer, as...
is the case of the QHE mentioned above, these properties may provide some advantages as regards device applications. For example, the rippling of BLG membranes was found to be weaker than that of SLG \cite{28,29}, meaning that the former can have an intrinsic mobility even higher than the latter.\footnote{Another limiting factor of electron mobility originates from the electrostatic coupling of carriers to the polarization field of the dielectric substrate, usually SiO\textsubscript{2} or SiC. This substrate limiting effect becomes important at room temperature in SLG but is sizably reduced in doped BLG \cite{31}.} Interestingly enough, strong suppression of electrical noise in BLG has been reported recently \cite{32} – a clear indication of a better screening of external disorder sources.

One of the most remarkable properties of BLG is the ability to open a gap in the spectrum by electric field effect – biased BLG. This has been shown both experimentally and theoretically, providing the first semiconductor with externally tunable gap\cite{33,34,35,36,37,38,39,40}. In the absence of external perpendicular electric field – unbiased BLG – the system is characterized by four bands, two of them touching each other at zero energy, and giving rise to the massive Dirac fermions mentioned above, and other two separated by an energy $\pm t_{\perp}$. Hence, an unbiased BLG is a two-dimensional zero-gap semiconductor $\perp$. At the neutrality point the conductance shows a minimum of the order of the conductance quantum $\hbar e^2/24\pi$\cite{13,21,31,32,41-44}. A property shared with SLG.\footnote{This prevents standard device applications where the presence of a finite gap producing high on-off current ratios is of paramount importance.} The fact that a simple perpendicular electric field is enough to open a gap, and even more remarkable, to control its size, clearly demonstrates the potential of this system for carbon-based electronics $\perp$\cite{45,46}.

The biased BLG reveals interesting properties on its own. The gap has shown to be robust in the presence of disorder\cite{47,48,49,50} induced either by impurities or dilution, but is completely absent in rotated (non AB-stacked) bilayers, where the SLG linear dispersion is recovered\cite{33,34,48}. The band structure near the gap shows a "Mexican-hat" like behavior, with a low doping Fermi surface which is a ring\cite{30}. Such a topologically nontrivial Fermi surface leads to an enhancement of electron-electron interactions, and to a ferromagnetic instability at low enough density of carriers\cite{55,56}. In the presence of a perpendicular magnetic field, the biased BLG shows cyclotron mass renormalization and an extra plateau at zero Hall conductivity, signaling the presence of a sizable gap at the neutrality point\cite{25,27,57}. Gaps can also be induced in stacks with more than two layers as long as the stacking order is of the rhombohedral-type\cite{36,38,39} although screening effects may become important in doped systems with increasing number of layers\cite{20}. Recently, a ferromagnetic proximity effect was proposed as a different mechanism which can also open a gap in the spectrum of the BLG, leading to a sizable magnetoresistive effect\cite{48}.

In this paper the electronic properties of a biased BLG are studied within a full tight-binding model, which enables the analysis of the whole bandwidth, validating previous results obtained using low-energy effective models. The electronic structure is computed both in the presence and in the absence of a perpendicular electric field. The screening of the applied perpendicular electric field is obtained within a self-consistent Hartree approach, and a comparison with experiments is provided. The effect of the bias in the cyclotron mass and Hall quantization is addressed, and the results are shown to agree well with experimental measurements. Zero energy surface states localized at zigzag edges in the presence of a perpendicular magnetic field are also studied, and the effect of the bias is considered.

The paper is organized as follows: in Sec. II the lattice structure of BLG and the tight-binding Hamiltonian are presented; bulk electronic properties are discussed in Sec. III both in the absence and presence of a finite bias, with particular emphasis on the screening correction; the effect of a perpendicular magnetic field is studied in Sec. IV. Sec. V contains our conclusions. We have also included three appendices: Appendix A provides details on the calculation of the density asymmetry between layers for a finite bias; in Appendix B we give the analytical expression for the biased BLG density of states, valid over the entire energy spectrum; analytical expressions for the cyclotron mass obtained within the full tight-binding model are given in Appendix C.

II. MODEL

The lattice structure of a bilayer is shown in Fig. 1. Here we consider only AB-Bernal stacking, where the top layer has its $A$ sublattice on top of sublattice $B$ of the bottom layer. We use indices 1 and 2 to label the top and bottom layer, respectively. As is clearly seen in Fig. 1 (right panel), the unit cell of a bilayer has twice the number of atoms of a single layer. The basis vectors may be written as,

$$a_1 = a \hat{e}_x, \quad a_2 = \frac{a}{2}(\hat{e}_x - \sqrt{3} \hat{e}_y),$$  \hspace{1cm} (2)

where $a = 2.46$ Å.
In the tight-binding approximation, the in-plane hopping energy, \( t \), and the inter-layer hopping energy, \( t_{\perp} \), define the most relevant energy scales (see Fig. 1). The simplest tight-binding Hamiltonian describing non-interacting \( \pi \)-electrons in BLG reads:

\[
H_{TB} = \sum_{i=1}^{2} H_i + t_{\perp} \sum_{\mathbf{R},\sigma} \left[ a_{i,\sigma}^\dagger(\mathbf{R})b_{i,\sigma}(\mathbf{R}) + \text{h.c.} \right] + H_V, \tag{3}
\]

with the SLG Hamiltonian

\[
H_i = -it \sum_{\mathbf{R},\sigma} \left[ a_{i,\sigma}^\dagger(\mathbf{R})b_{i,\sigma}(\mathbf{R}) + a_{i,\sigma}(\mathbf{R})b_{i,\sigma}(\mathbf{R} - \mathbf{a}_1) \right] + a_{i,\sigma}^\dagger(\mathbf{R})b_{i,\sigma}(\mathbf{R} - \mathbf{a}_2) + \text{h.c.}, \tag{4}
\]

where \( a_{i,\sigma}(\mathbf{R}) \) \( [b_{i,\sigma}(\mathbf{R})] \) is the annihilation operator for electrons at position \( \mathbf{R} \) in sublattice \( A_i \) (\( B_i \)), \( i = 1, 2 \), and spin \( \sigma \). The in-plane hopping \( t \) can be inferred from the Fermi velocity in graphene \( v_F = e\hbar k_F / m_e \approx 10^6 \text{m/s} \) yielding \( t \approx 3.1 \text{eV} \), in good agreement with what is found experimentally for graphite. This value also agrees with a recent Raman scattering study of the electronic structure of BLG. As regards the inter-layer hopping \( t_{\perp} \), angle-resolved photoemission spectroscopy (ARPES) measurements in epitaxial BLG give \( t_{\perp} \approx 0.43 \text{eV} \) and Raman scattering for BLG obtained by micro-mechanical cleavage of graphite yields \( t_{\perp} \approx 0.30 \text{eV} \). The experimental value for bulk graphite is \( t_{\perp} \approx 0.39 \text{eV} \) which means that for practical purposes we can always assume \( t_{\perp} / t \sim 0.1 \ll 1 \). These values for \( t \) and \( t_{\perp} \) compare fairly well with what is obtained from first-principles calculations for graphite using the well-established Slonczewski-Weiss-McClure (SWM) parametrization models to fit the bands near the Fermi energy. The SWM model assumes extra parameters that can also be incorporated in a tight-binding model for BLG. Namely, the inter-layer second-NN hoppings \( \gamma_3 \) and \( \gamma_4 \), where \( \gamma_3 \) connects different sublattices \( (B_1 - A_2) \) and \( \gamma_4 \) equal sublattices \( (A_1 - A_2) \) and \( B_1 - B_2 \). Additionally, there is an on-site energy \( \Delta \) reflecting the inequivalence between sublattices \( A_1, B_2 \) and \( B_1, A_2 \) — the former project exactly on top of each other while the latter lay on the hexagon center of the other layer. The consequences of these extra terms for the band structure obtained from Eq. (3) are well known: \( \gamma_3 \) induces trigonal warping and both \( \gamma_4 \) and \( \Delta \) give rise to electron-hole asymmetry. Their values, however, are less well known in BLG than in bulk graphite. For graphite we have \( \gamma_3 \approx 0.315 \text{eV} \) and \( \gamma_4 \approx 0.044 \text{eV} \) while in BLG the first seems to be three times smaller and the second three times larger \( \gamma_3 \approx 0.10 \text{eV} \) and \( \gamma_4 \approx 0.12 \text{eV} \). As regards the on-site energy \( \Delta \), it is found to be small and negative in graphite \( \Delta \approx -0.008 \text{eV} \) while there is an indication that in BLG it is positive \( \Delta \approx 0.018 \text{eV} \). The in-plane second-NN hopping energy \( t' \) is not considered in the usual tight-binding parametrization of the SWM model. Nevertheless, this term can have important consequences since it breaks particle-hole symmetry but does not modify the Dirac spectrum. It is expected to be of the order \( t' \approx 0.12 \text{eV} \), as obtained by fitting ab initio results. Here we keep the model as simple as possible by neglecting \( t', \gamma_3, \gamma_4, \) and \( \Delta \), unless otherwise stated.

We are interested in the properties of BLG in the presence of a perpendicular electric field — the biased BLG. The external perpendicular electric field gives rise to an electrostatic energy difference between the two layers, which we parametrize by \( V \). The effect of this energy difference between layers may be accounted for by \( H_V \) in Eq. (3) with \( H_V \) given by

\[
H_V = \frac{V}{2} \sum_{\mathbf{R},\sigma} \left[ n_{A1}(\mathbf{R}) + n_{B1}(\mathbf{R}) - n_{A2}(\mathbf{R}) - n_{B2}(\mathbf{R}) \right], \tag{5}
\]

where \( n_{A1}(\mathbf{R}) \) and \( n_{B1}(\mathbf{R}) \) are number operators.

When a perpendicular magnetic field \( \mathbf{B} = B \mathbf{z} \) is applied to the system \( t_{\perp} \) is unaffected but \( t \) acquires a phase \( e^{i\phi B \cdot \mathbf{R}} \) such that \( t \rightarrow t e^{i\phi} B^k A^{k+1} \mathbf{R} \cdot d\mathbf{r} \), where \( e \) is the electron charge, \( \delta \) is a vector NN sites, and \( A \) is the vector potential (we use units such that \( c = 1 = \hbar \)).

### III. BULK ELECTRONIC PROPERTIES

The bulk properties of the model defined by Eq. (3) can be determined by imposing periodic boundary conditions and applying the Fourier transformation, as in any system with translational invariance. Introducing the Fourier components \( a_{i,\sigma,k} \) and \( b_{i,\sigma,k} \) of operators \( a_{i,\sigma}(\mathbf{R}) \) and \( b_{i,\sigma}(\mathbf{R}) \), respectively, with the layer index \( i = 1, 2 \), we can rewrite Eq. (3) as

\[
H = \sum_{k,\sigma} \psi_{\sigma,k}^\dagger H_k \psi_{\sigma,k}, \tag{6}
\]

where \( \psi_{\sigma,k} = [b_{1,\sigma,k}^\dagger, a_{1,\sigma,k}^\dagger, a_{2,\sigma,k}^\dagger, b_{2,\sigma,k}^\dagger] \) is a four component spinor, and \( H_k \) is given by

\[
H_k = \begin{pmatrix}
V/2 & -t_{sk} & 0 & -t_{\perp} \\
-t_{sk}^* & V/2 & 0 & 0 \\
0 & 0 & -V/2 & -t_{sk} \\
0 & -t_{sk}^* & V/2 & -V/2
\end{pmatrix}. \tag{7}
\]

The factor \( s_k \) determines the matrix elements for the SLG Hamiltonian in reciprocal space \( (t_{\perp} = 0, V = 0) \),

\[
s_k = 1 + e^{ik \mathbf{a}_1} + e^{ik \mathbf{a}_2}, \tag{8}
\]

from which the SLG dispersion is obtained,

\[
e_{k}/t = \pm|s_k|
\]

\[
= \pm \left[ 3 + 2 \cos(a_{x}k_x) + 4 \cos(a_{x}/2) \cos \left( a_{y} \sqrt{3}/2 \right) \right]^{1/2}. \tag{9}
\]
The conduction (+) and valence (−) bands represented by Eq. 2 touch each other in a conical way at the corners of the first BZ, the K and K' points in the right panel of Fig. 2. This touching occurs at zero energy, the Fermi energy for undoped graphene. At low energies (|k| ≪ |t|) Eq. 3 reduces to the linear dispersion relation given in Eq. 1. The continuum approximation for Eq. 7 may then be obtained by introducing the wave vector q which measures the difference between k and the corners of the BZ. Near the K points Eq. 6 reads

$$H_{k} = \begin{pmatrix} V/2 & v_F p e^{-i\varphi_p} & 0 & -t_\perp \\ v_F p e^{i\varphi_p} & V/2 & 0 & 0 \\ 0 & 0 & -V/2 & -v_F p e^{-i\varphi_p} \\ 0 & 0 & v_F p e^{i\varphi_p} & -V/2 \end{pmatrix},$$

where p = hq and \(\varphi_p = \tan^{-1}(p_y/p_x)\). Around the K' points Eq. 10 with complex conjugate matrix elements defines \(H_{k'}\).

Equation (10) can be further simplified if one assumes \(v_F p, V \ll t_\perp\). By eliminating high energy states perturbatively we can write a two-band effective Hamiltonian describing low-energy states whose electronic amplitude is mostly localized on B1 and A2 sites. Near the K points the result of Hamiltonian may be written as

$$H_{\text{eff}} = -\begin{pmatrix} -V/2 & 0 & e^{-i\varphi_p} p e^{2i\varphi_p}/t_\perp \\ 0 & V/2 & 0 \\ e^{i\varphi_p} p e^{-2i\varphi_p}/t_\perp & 0 & -V/2 \end{pmatrix},$$

whereas the complex conjugate matrix elements should be taken for a low-energy description around the K' points. The two-component wave functions have the form \(\Phi = (\phi_{B1}, \phi_{A2})\).

In the following we discuss the electronic structure resulting from the tight-binding Hamiltonian (9), and comment on the approximations given above by Eqs. 10 and 11.

### A. Unbiased bilayer

In the absence of applied perpendicular electric field (the bias) the system has four bands given by

$$E_{k}^{\pm} = \pm \sqrt{\epsilon_k^2 + t_\perp^2/4} \pm t_\perp/2,$$

where \(\epsilon_k\) is the dispersion of a SLG as given in Eq. 2. The band structure defined by Eq. 13 is shown in Fig. 2.

Undoped BLG has exactly one electron per \(\pi\) orbital, that is, it is a half-filled system. In this case the chemical potential crosses exactly at the K and K' points (the Dirac points) at the corners of the BZ. At these corners the dispersion is parabolic, as shown in the inset of Fig. 2. Indeed, expanding Eq. 13 around the two inequivalent corners, \(aK' = (4\pi/3, 0) = -aK\), we get,

$$E^{\pm}(p) \approx \pm \sqrt{v_F^2 p^2 + t_\perp^2/4} \approx \pm (v_F^2 p^2/2 + t_\perp^2/2) \pm t_\perp/2, \quad (13)$$

with \(p = hq\) as in Eq. 10, where \(q\) measures the distance relatively to the Dirac points. Note that, in the first approximation in Eq. 13, we have just obtained the eigenvalues of the Hamiltonian in the continuum approximation, for \(V = 0\), as given in Eq. 10. The near zero energy dispersion in the second approximation in Eq. 13, \(E(p) \approx \pm v_F^2 p^2/2\), represents the eigenvalues of the two-band effective Hamiltonian in Eq. 11. The low-energy quasiparticles are massive, with a light effective mass given by \(m^* = t_\perp/(2v_F^2) \approx 0.03m_e\), where \(m_e\) is the bare electron mass.

The spectrum of a graphene bilayer can also be obtained from decoupled graphene layers. The operators that diagonalize the decoupled layers can be written as,

$$e_{1,\sigma,k} = \frac{1}{\sqrt{2}} \left( e^{i\delta_k/2} a_{1,\sigma,k} - e^{-i\delta_k/2} b_{1,\sigma,k} \right), \quad (14)$$

$$h_{1,\sigma,k} = \frac{1}{\sqrt{2}} \left( e^{i\delta_k/2} a_{1,\sigma,k} + e^{-i\delta_k/2} b_{1,\sigma,k} \right), \quad (15)$$

$$e_{2,\sigma,k} = \frac{1}{\sqrt{2}} \left( e^{i\delta_k/2} a_{2,\sigma,k} - e^{-i\delta_k/2} b_{2,\sigma,k} \right), \quad (16)$$

$$h_{2,\sigma,k} = \frac{1}{\sqrt{2}} \left( e^{i\delta_k/2} a_{2,\sigma,k} + e^{-i\delta_k/2} b_{2,\sigma,k} \right), \quad (17)$$

where \(e\) and \(h\) stand for electron and hole states in Eq. 9, respectively. The phase \(\delta_k\) is given by \(\delta_k = \tan^{-1}(3s_k/\bar{R}s_k)\), with \(s_k\) as in Eq. 8, and operators \(a_{1,\sigma,k}\) and \(b_{1,\sigma,k}\) as in Eq. 6. When written in terms of band operators given in Eqs. 14, 17, the inter-layer coupling term reads,

$$H_{12} = \frac{t_\perp}{2} \sum_{k,\sigma} \left( e_{1,\sigma,k}^{\dagger} e_{2,\sigma,k} + e_{1,\sigma,k}^{\dagger} h_{2,\sigma,k} ight) + h_{1,\sigma,k}^{\dagger} e_{2,\sigma,k} + h_{1,\sigma,k}^{\dagger} h_{2,\sigma,k} + \text{h.c.} \quad (18)$$

Equation (18) describes a 4-site tight-binding problem, where there are two degenerate states (\(\pm v_F/2\) Bloch states) of zero energy, one of energy \(-t_\perp\) (0 Bloch state), and a fourth state at \(+t_\perp\) (\(\pm v_F/2\) Bloch state). These are essentially the four states at the corners of the BZ \(p = 0\) in
Eq. [12]. For other \( k \)-values the electron and hole states are no longer degenerate, showing an energy separation of \( 2\epsilon_k \). However, the electron (hole) states of the two decoupled layers remain degenerate. For \( 2\epsilon_k > t_\perp \), one obtains a coupling \( t_\perp/2 \) between \( e_1 \) and \( e_2 \) degenerate electron bands, as well as between \( h_1 \) and \( h_2 \) hole bands. The inter-layer term \( H_{12} \) splits these two pairs of bands by \( t_\perp \), whereas the coupling between \( e \) and \( h \) bands is suppressed by a \( t_\perp/2\epsilon_k \) factor.

**B. Biased bilayer**

Now we address the electronic structure of the biased BLG using the full tight-binding Hamiltonian given by Eq. [3]. The spectrum of Eq. [3] for \( V \neq 0 \) reads:

\[
E_k^\pm(V) = \pm \sqrt{\epsilon_k^2 + \frac{t_\perp^2}{4} + \frac{V^2}{4} \pm \sqrt{\frac{t_\perp^4}{16} + \left( \frac{t_\perp^2}{4} + \frac{V^2}{4} \right)^2}}.
\]  

(19)

The resulting band structure is shown in Fig. 3(a). As can be seen from Eq. [12], the \( V = 0 \) gapless system turns into a semiconductor with a gap controlled by \( V \). Moreover, the two bands close to zero energy are deformed near the corners of the BZ [inset of Fig. 3(a)], so that the minimum of \( |E_k^\pm(V)| \) no longer occurs at these corners. As a consequence, the lowest doping Fermi surface is completely different from the \( V = 0 \) case, with its shape controlled by \( V \).

It can be readily shown that the minimum of sub-band \( E_k^\pm(V) \) for \( k \approx 0 \) occurs for all \( k \)'s satisfying

\[
\epsilon_k^2 = \alpha(V, t_\perp),
\]

(20)

with \( \alpha(V, t_\perp) = \left( \frac{V^4}{4} + \frac{t_\perp^2 V^2}{4} + 2 t_\perp^4 / 2 \right) / (V^2 + t_\perp^2) \) – note that \( \partial E_k^\pm / \partial \epsilon_k = 0 \) at the desired extrema. Equation (20) has solutions for \( \sqrt{\alpha} \leq 3t \) (3t is half of the single layer bandwidth). When \( \sqrt{\alpha} > 3t \) the minimum of \( E_k^\pm(V) \) occurs at the \( \Gamma \) point. Figure 3(b) shows the solution of Eq. (20) around the \( K \) point for \( V = t_\perp/2, 2t_\perp, 4t_\perp \) (around the \( K' \) point the figure is rotated by \( \pi/3 \)). At low doping the Fermi sea acquires a line shape given by the solution of Eq. (20), the line width being determined by the doping level. As can be seen in Fig. 3(b), when \( V < t_\perp \) the Fermi sea approaches a ring, the Fermi ring, centered at the BZ corner. As \( V \) is increased there is an apparent trigonal distortion showing up, which originates from the single layer dispersion in Eq. (20).

The existence of a Fermi ring is easily understood using the continuum version of Eq. (19), i.e., the eigenvalues of Eq. (10). This amounts to substitute the single layer dispersion in Eq. (19) by \( v_F p \), which immediately implies cylindrical symmetry around \( K \) and \( K' \). If we further assume that \( v_F p \ll t_\perp \), Eq. (19) is then well approximated by the “Mexican hat” dispersion

\[
E^\pm(V) \approx \pm \frac{V}{2} + \frac{\epsilon_k^2}{2t_\perp^2} p^2 \pm \frac{\epsilon_k^4}{2t_\perp^4} p^4,
\]

(21)

which explains the Fermi ring. If, instead, we have \( V < v_F p \ll t_\perp \), we can approximate Eq. (19) by

\[
E^\pm(V) \approx \pm \sqrt{V^2/4 + v_F^2 p^4/t_\perp^4},
\]

(22)

which corresponds exactly to the eigenvalues of the effective two-band Hamiltonian in Eq. (11). Note that no continuum approximation can produce the trigonal distortion shown in Fig. 3(b). In fact, around the \( K \) point and setting \( k_y = 0 \), the solutions of Eq. (20) are

\[
q_{x,1} = \frac{4\pi}{3} - 2 \arccos\left(\frac{-1}{\alpha}\right)/2, \quad q_{x,2} = \frac{4\pi}{3} - 2 \arccos\left(\frac{1}{\alpha}\right)/2,
\]

(23)

where \( q_{x,i} \) is the position of the two minima along the \( k_x \) direction relatively to the \( K \) point. It is clearly seen from Eqs. (23) and (24) that for \( \alpha \leq 1 \) the position of the two minima is asymmetric relatively to the Dirac point, with \( |q_{x,1}| < |q_{x,2}| \).

The gap between conduction and valence bands, \( \Delta_g \), is twice the minimum value of \( E_k^\pm(V) \) due to electron-hole symmetry, and is given by

\[
\Delta_g = \begin{cases} \sqrt{t_\perp^2 V^2 / (t_\perp^4 + V^2)} & V \leq V_c \\ 2t \sqrt{9 + \frac{t_\perp^2 V^2}{V_c^2} - \frac{V^4}{4 V_c^2} + 9 \frac{t_\perp^4 + V^2}{t_\perp^4}} & V > V_c \end{cases},
\]

(25)

where \( V_c = 18(2^2 - t_\perp^2 + t_\perp^4 + t_\perp^4)^{1/2} / 2 \approx 6t \), the approximation being valid for \( t_\perp \ll t \). Note that \( V \) parametrizes the effect of a perpendicular electric field, and therefore can be controlled externally. This means, as a consequence of Eq. (20), that the biased BLG is a semiconductor with a gap that can be tuned externally by electric field. From Eq. (25) it can be seen that for both \( V \ll t_\perp \) and \( V \gg t \) one finds \( \Delta_g \approx V \). However, there is a region for \( t_\perp \ll V \ll 6t \) where the gap shows a
plateau $\Delta_g \sim t_\perp$, as depicted in Fig. 3(c). The plateau ends when $V \approx 6t$ (not shown).

This behavior is easily understood from the point of view of decoupled layers plus a 4-site tight-binding problem [Eq. (15)]. For the unbiased bilayer the two degenerate eigenstates $\psi_+$ and $\psi_-$ of Eq. (15), the so-called $\pm \pi/2$ Bloch states, are given in terms of band operators as,

$$\psi_\pm = \frac{1}{\sqrt{2}} (e^{i\mp \pi/2} e_2 - h_1 + e^{\mp \pi/2} h_2)$$

$$= \frac{1}{\sqrt{2}} (-e^{-i\delta/2} h_1 + e^{i\delta/2} a_2), \quad (26)$$

where momentum and spin indices have been omitted. For $V \ll t_\perp$, near the Dirac points, the bias acts as a perturbation, coupling the two zero energy states $\psi_\pm$. Only the non-diagonal matrix element is non-zero and equal to $V/2$. So the splitting, and the gap, is in this limit,

$$\Delta_g = V + O\left(\frac{V}{t_\perp}\right), \quad V \ll t_\perp. \quad (27)$$

The case $V > t_\perp$ is also completely unveiled within this framework. For the decoupled layers in the presence of a bias we can readily see that there are values of $k$ for which the hole band of layer 1 crosses the electron band of layer 2. At values of $k$ such that,

$$2\epsilon_k = V, \quad (28)$$

which is just Eq. (20) for $t_\perp = 0$, the coupling term given by Eq. (15) couples four states of energies $-|\epsilon_k| - V$, $-|\epsilon_k| + V = |\epsilon_k| - V$, and $|\epsilon_k| + V$. For $t_\perp \ll \epsilon_k$ the effect of $H_{12}$ is to lift the degeneracy of the two middle states. Since the coupling between them is $t_\perp/2$, the gap between these states is $t_\perp$. This explains the origin of the plateau in Fig. 3. As $V$ changes, the $k$-values where the bands $h_1$ and $e_2$ are degenerate move in momentum space [Eq. (28)], but the gap remains,

$$\Delta_g = t_\perp + O\left(\frac{t_\perp^2}{V} + \frac{t_\perp^2}{\epsilon_k}\right), \quad t_\perp \ll V \leq 6t. \quad (29)$$

At $V = 6t$, which is the $V_c$ value separating the two regimes in Eq. (25) (for $t_\perp \ll t$), the bands no longer cross. The gap occurs at the $\Gamma$ point between the $h_1$ and $e_2$ bands, which are now very weakly coupled, so that,

$$\Delta_g = V - 6t + O\left(\frac{t_\perp^2}{V - 6t}\right), \quad V > 6t. \quad (30)$$

It is worth mentioning that experimentally $V \ll t$ always hold, as larger bias values would imply huge unsustainable electric fields due to the small separation between the two graphene layers in BLG. This means that the relation between the gap $\Delta_g$ and the parameter $V$ is always given, for practical purposes, by the first expression in Eq. (25).

C. Screening of the external field

So far we have considered $V$, i.e. the electrostatic energy difference between layers felt by a single electron, as a band parameter that controls the $g_p$. However, the parameter $V$ can be related with the perpendicular electric field applied to BLG, avoiding the introduction of an extra free parameter in the present theory.

Let us call $E = E\partial_z$ the perpendicular electric field felt by electrons in BLG. The corresponding electrostatic energy $U(z)$ for an electron of charge $-e$ is related to the electric field as $eE = \partial U(z)/\partial z$, and thus $V$ is given by

$$V = U(z_1) - U(z_2) = eEd, \quad (31)$$

where $z_1$ and $z_2$ are the positions of layer 1 and 2, respectively, and $d \equiv z_1 - z_2 = 3.4$ Å is the inter-layer distance. Given the experimental conditions, the value of $E$ can be calculated under a few assumptions, as detailed in the following.

1. External field in real systems

If we assume the electric field $E$ in Eq. (31) to be due exclusively to the external electric field applied to BLG, $E = E_{ext}$, all we need in order to know $V$ is the value of $E_{ext}$,

$$V = eE_{ext}d. \quad (32)$$

The experimental realization of a biased BLG has been achieved in epitaxial BLG through chemical doping, and in back gated exfoliated BLG. In either case the value of $E_{ext}$ can be extracted assuming a simple parallel plate capacitor model.

In the case of exfoliated BLG, devices are prepared by micromechanical cleavage of graphite on top of an oxidized silicon wafer (300 nm of $SiO_2$), as shown in the left panel of Fig. 4(a). A back gate voltage $V_g$ applied between the sample and the Si wafer induces charge carriers due to the electric field effect, resulting in carrier densities $n_g = \beta V_g$ relatively to half-filling ($n_g > 0$ for electrons and $n_g < 0$ for holes). The geometry of the resulting capacitor determines the coefficient $\beta$. In particular, the electric field inside the oxidized layer is $E_{ox} = e\eta/(SiO_2 \varepsilon_0)$, where $SiO_2$ and $\varepsilon_0$ are the permittivities of $SiO_2$ and free space, respectively. This implies a gate voltage $V_g = e\eta/(SiO_2 \varepsilon_0)$, from which we obtain the coefficient $\beta = \varepsilon SiO_2 \varepsilon_0/(\varepsilon t)$. For a $SiO_2$ thickness $t = 300$ nm and a dielectric constant $SiO_2 = 3.9$ we obtain $\beta \approx 7.2 \times 10^{10}$ cm$^{-2}$/V, which is in agreement with the values found experimentally. In order to control independently the $g_p$ value and the Fermi level, in Ref. 33 the devices have been chemically doped by deposition of NH$_3$ on top of the upper layer, which adsorbs on graphene and effectively acted as a top gate providing a fixed electron density $n_0$. Charge conservation then
implies a total density \( n \) in BLG given by \( n = n_g + n_0 \), or in terms of the applied gate voltage,

\[
n = \beta V_g + n_0.
\]  

(33)

In Fig. 4(b) the charge density in BLG is shown as a function of \( V_g \). The symbols are the experimental result obtained from Hall effect measurements and the line is a linear fit with Eq. (33). The fit provides \( n_0 \), which for this particular experimental realization is \( n_0 \approx 1.8 \times 10^{12} \text{ cm}^{-2} \), and validates the parallel plate capacitor model applied to the back gate, since the fitted \( \beta \approx 7.2 \times 10^{10} \text{ cm}^{-2}/\text{V} \) is in excellent agreement with the theoretical value. Extending the parallel plate capacitor model to include the effect of dopants, the external field \( E_{\text{ext}} \) is the result of charged surfaces placed above and below BLG. The accumulation or depletion layer in the Si wafer contributes with an electric field \( E_0 = \varepsilon_0 n_g/(2\varepsilon \varepsilon_0) \), while dopants above BLG effectively provide the second charged surface with electric field \( E_1 = -\varepsilon_0 n_a/(2\varepsilon \varepsilon_0) \). A relative dielectric constant \( \varepsilon_r \) different from unity may be attributed to the presence of SiO\(_2\) below and vacuum on top, which gives \( \varepsilon_r \approx (\varepsilon_{\text{SiO}_2} + 1)/2 \approx 2.5 \), a value that can be slightly different due to sorption of water molecules. Adding the two contributions, \( E_{\text{ext}} = E_0 + E_1 \), and making use of the charge conservation relation, we arrive at an electrostatic energy difference \( V \) [Eq. (32)] that depends linearly on the BLG density,

\[
V = \left( \frac{n}{n_0} - 2 \right) \frac{\varepsilon_0 n_a d}{2 \varepsilon \varepsilon_0}.
\]  

(34)

In treating the dopants as a homogeneous charged layer we ignore possible lattice distortion induced by adsorbed molecules, as well as the electric field due to the NH\(_3\) electric dipole, which may contribute to the gap in the spectrum. However, it has been shown recently that for NH\(_3\) these effects counteract, giving rise to a much smaller gap than other dopant molecules as for instance NH\(_2\) and CH\(_3\). For the biased BLG realized in Ref. 34, independence of Fermi level and carrier density was achieved with a real top gate, which makes the parallel plate capacitor model a suitable approximation in that case.

In the case of epitaxial BLG, devices are grown on SiC by thermal decomposition. The substrate is fixed (SiC), and graphene behavior develops for carbon layers above the buffer layer as schematically shown in the right panel of Fig. 1(a). Due to charge transfer from substrate to film, the as-prepared BLG devices appear electron doped with density \( n_a \). The substrate’s depletion layer provides the external electric field necessary to make the system a biased BLG. In Ref. 33 the BLG density \( n \) was varied by doping the system with potassium (K) on top of the upper layer [see Fig. 4(a)], which originates an additional charged layer contributing to the external electric field. Applying the same parallel plate capacitor model as before, we get an electrostatic energy difference that can be written as

\[
V = \left( \frac{n}{n_0} - 2 \right) \frac{\varepsilon_0 n_a d}{2 \varepsilon \varepsilon_0}.
\]  

(35)

Following a similar reasoning to the case of exfoliated graphene on top of SiO\(_2\), we would write \( \varepsilon_r \approx (\varepsilon_{\text{SiC}} + 1)/2 \approx 5 \). However, this value should not be taken too seriously, as it neglects completely the presence of the buffer layer. In Fig. 4(c) we compare Eq. (35) with experimental results for \( V \) obtained by fitting ARPES measurements from Ref. 33. For this particular biased BLG realization, the as-prepared carrier density was \( n_a \approx 10^{13} \text{ cm}^{-2} \). From Eq. (35), this \( n_a \) value implies a zero \( V \), i.e., zero electric field and therefore zero gap, for the bilayer density \( n^{\text{th}} \approx 2 \times 10^{13} \text{ cm}^{-2} \). Experimentally, a zero gap was found around \( n^{\exp} \approx 2.3 \times 10^{13} \text{ cm}^{-2} \). Given the simplicity of the theory, it can be said that \( n^{\text{th}} \) and \( n^{\exp} \) are in good agreement. However, the agreement is only good at \( V \approx 0 \), since the measured \( V \) is not a linear function of \( n \), as Eq. (35) implies. In what follows we analyze in detail the effect of screening and how it modifies Eqs. (34) and (35).

2. Screening correction

In deriving Eqs. (34) and (35) we assumed that the electric field \( E \) in the BLG region was exactly the external one, \( E_{\text{ext}} \). There is, however, an obvious additional contribution: the external electric field polarizes the BLG, inducing some charge asymmetry between the two graphene layers, which in turn give rise to an internal electric field, \( E_{\text{int}} \), that screens the external one.

To estimate \( E_{\text{int}} \) we can again apply a parallel plate capacitor model. The internal electric field due to the charge asymmetry between planes may thus be written
where \( -e \Delta n \) is the induced charge imbalance between layers, which can be estimated through the weight of the wave functions in each layer,

\[
\Delta n = n_1 - n_2 = \frac{2}{N_c A_0} \sum_{j,l=\pm} \sum_k \left( |\varphi_{A1,k}^j|^2 + |\varphi_{B1,k}^j|^2 - |\varphi_{A2,k}^j|^2 - |\varphi_{B2,k}^j|^2 \right),
\]

(37)

where the factor 2 comes from spin degeneracy, \( N_c \) is the number of unit cells and \( A_0 = a^2 \sqrt{3}/2 \) is the unit cell area, \( jl \) is a band label, and the prime sum runs over all occupied \( k \)’s in the Brillouin zone defined in Fig. 2. The amplitudes \( \varphi_{A1,k}^j \) and \( \varphi_{B1,k}^j \) with \( i = 1, 2 \), are determined by diagonalization of Eq. (2), enabling \( \Delta n \) to be written as

\[
\Delta n = \frac{2}{N_c A_0} \sum_{j,l=\pm} \sum_k \left( (\epsilon_k^2 + K_{k,j}^{B1})(\epsilon_k^2 - K_{k,j}^{B1}) - (\epsilon_k^2 + K_{k,j}^{A1})(\epsilon_k^2 - K_{k,j}^{A1}) \right) \frac{1}{2} K_{k,j}^{B1},
\]

(38)

where \( \epsilon_k \) is given by Eq. (9), \( K_{k,j}^{B1} = (V/2 ± E_k^j)^2 \) with \( E_k^j \) given by Eq. (15). Taking the limit \( N_c \to \infty \), it is possible to write Eq. (35) as an energy integral weighted by the density of states of SLG, as described in Appendix A. What is important to note is that in order to calculate \( \Delta n \) we must specify \( V \), as it appears in the integral kernel on the right hand side of Eq. (35), and the carrier density \( n \), from which we get the occupied \( k \)’s. On the other hand, \( \Delta n \) determines \( E_{int} \) through Eq. (36), and in turn \( E_{int} \) enters Eq. (31) through \( E \) to give \( V \). Thus, a self-consistent procedure must be followed to calculate the screened energy difference between layers \( V \). In particular, for the two experimental realizations of biased BLG discussed in Sec. III C 1, the self-consistent equation that determines \( V \) reads: in the case of exfoliated BLG

\[
V = \left[ \frac{n}{n_0} - 2 + \frac{\Delta n(n,V)}{n_0} \right] \frac{\epsilon^2 n_0 d}{2e\varepsilon_0},
\]

(39)

in the case of epitaxial BLG

\[
V = \left[ 2 - \frac{n}{n_a} + \frac{\Delta n(n,V)}{n_a} \right] \frac{\epsilon^2 n_0 d}{2e\varepsilon_0}.
\]

(40)

The self-consistent electric field \( E = E_{ext} + E_{int} \) at the BLG region, with \( E_{int} \) given by Eq. (40) for \( \varepsilon_r = 1 \), is shown at half-filling as a function of \( E_{ext} \) in Fig. 3(a). The screened \( E \) is approximately a linear function of \( E_{ext} \), with a constant of proportionality that depends on the specific value of \( t_\perp \). Increasing \( t_\perp \) leads to an increased screening, which can be understood as due to an increased charge imbalance between layers, as shown in Fig. 3(b). The highly non-linear effect of inducing a finite carrier density \( n \neq 0 \) can be seen in the insets of Fig. 3(a) and 3(b), for \( t_\perp = 0.1f \) and \( E_{ext} = 0.3 \) V/nm.

As a validation test to the present self-consistent treatment, we compare Eq. (40) with experimental results for \( V \) obtained by fitting ARPES measurements from Ref. 33, as mentioned in Sec. III C 1. The result is shown in Fig. 3(c). Clearly, the self-consistent \( V \) given by Eq. (40) for \( \varepsilon_r = 1 \) is a much better approximation than the unscreened result of Eq. (35) [see Fig. 3(c)]. The best fit is obtained for \( \varepsilon_r \sim 1 - 2 \), as can be seen in the inset of Fig. 3(c). The value \( \varepsilon_r \) is \( (\varepsilon_r + 1)/2 \approx 5 \) is too high, possibly because of the presence of the so-called buffer layer. Note, however, that the dielectric constant \( \varepsilon_r \) may effectively be tuned externally, as recently shown in SLG by adding a water overlay in ultra-high vacuum. In Fig. 3(d) we show the gap \( \Delta_g \) as a function of carrier density \( n \) for the biased BLG device shown in the left panel of Fig. 3(a), with realistic values of chemical doping \( n_0 \). The gap is given by Eq. (29), with \( t_\perp \approx 0.22 \) eV and \( V \) obtained by solving self-consistently Eq. (39) for

\[
E_{int} = \frac{e\Delta n}{2e\varepsilon_0}.
\]

(36)
\( \varepsilon_r = 1 \). Note that for \( E_{\text{ext}} = 0 \) we always have \( E_{\text{ext}} = 0 \) (the charge imbalance must be externally induced), and therefore we also have \( V = 0 \) and \( \Delta_q = 0 \). For this particular biased BLG device the present model predicts \( E_{\text{ext}} = 0 \) for \( n = 2n_0 \), which explains the asymmetry for \( \Delta_q \) vs \( n \) shown in Fig. 5(d). Note also that this device effectively provides a tunable gap semiconductor, as implied by Fig. 5(d): different gap values are achieved by tuning the gate voltage \( V_g \), which controls the carrier density \( n \) through Eq. (33).

The most important characteristic of such devices, from the point of view of applications, is the maximum size of the gap which could be induced. The maximum \( \Delta_q \) occurs when \( V_g \) reaches its maximum, which occurs just before the breakdown of SiO₂. The breakdown field for SiO₂ is \( \gtrsim 1 \) V/\( \mu \)m, meaning that \( V_g \) values as high as 300 V are possible for the device shown in the left panel of Fig. 4(a). From Eq. (33) we see that \( V_g \approx \pm 300 \) V implies \( n - n_0 = \pm 22 \times 10^{12} \) cm\(^{-2} \), and therefore Fig. 5(d) nearly spans the interval of possible densities. It is apparent, specially for \( n_0 = 5.4 \times 10^{12} \) cm\(^{-2} \), that when the maximum allowed densities are reached the gap seems to be approaching a saturation limit. This saturation is easily identified with the plateaus shown in Fig. 3(c) for \( \Delta_q \) vs \( V_g \), occurring for \( V_g \gtrsim t_\perp \). We may then conclude that such devices enable the entire range of allowed gaps (up to \( t_\perp \)) to be accessed. The effect of using a different dielectric constant (\( \varepsilon_r = 2 \)) is shown as a full line in the left inset of Fig. 5(d), and the result for the unscreened case in the right inset, both for \( n_0 = 5.4 \times 10^{12} \) cm\(^{-2} \). The former makes the gap slightly smaller, and the last slightly larger, but the main conclusions remain.

It is worth noting that the screening correction expressed in Eq. (23) leads to a term in the Hamiltonian which is exactly the Hartree correction due to the charge asymmetry between layers. This approach has been followed in Refs. 38 and 39, in the continuum approximation, and has been tested against \textit{ab initio} calculations at half-filling in Ref. 38. The agreement between the self-consistent Hartree corrected potential difference \( V \) and that obtained by fitting the density functional theory (DFT) energy bands is generally good, although DFT in Ref. 38 predicts a slightly larger screening effect, particularly for smaller external electric fields. It should be mentioned, however, that in Ref. 39 a different \textit{ab initio} calculation has shown a slightly smaller screening than the self-consistent Hartree approach. The discrepancy between the DFT results of Refs. 38 and 39 is probably due to the different approximation for exchange-correlation potential, \textit{generalized gradient approximation} in the former and \textit{local density approximation} in the later.

3. Screening in continuum models

The self consistent Hartree approach considered in the previous section has been applied to the full tight-binding Hamiltonian given in Eq. (3). Here we compare the results for the potential difference \( V \) and gap \( \Delta_q \) when the screening correction is used within the continuum approximation, either for the 4-band model of Eq. (10) or for the 2-band model of Eq. (11). This self consistent Hartree approach in the continuum has been followed in Refs. 33, 34.

Here we concentrate on the device shown in the left panel of Fig. 1(a), whose self consistent equation for \( V \) given by Eq. (23). This self consistent expression for \( V \) remains the same in both the 4-band and the 2-band models. The difference with respect to the full tight-binding result is the way the layer asymmetry \( \Delta \) and the gap are determined.

In the case of the 4-band model, \( \Delta \) is still given by Eq. (33), with the substitutions \( \epsilon_r \rightarrow \epsilon_r n \) and

\[
\sum_{j,l=\pm} \sum_{k} \int_{0}^{2\pi} \int_{0}^{2\pi} f_{p}^{2} \, dp, \quad \text{where the prime on the right band summation means sum over total or partially occupied bands. Depending on the band in question and the value of the Fermi energy \( E_F \), the limits of integration are \( p_1, p_2 = (0, \pm, \Lambda) \), where}
\]

\[
v_{p}^{\pm} = \sqrt{E_{F}^{2} + V^{2}/4 \pm \sqrt{E_{F}^{2} + V^{2}/4}}/4,
\]

and \( \Lambda \) is a BZ cutoff that can be chosen such that

\[
\frac{4}{\pi^{2}} \int_{0}^{2\pi} \int_{0}^{2\pi} dp \quad \text{and} \quad \Lambda = \hbar \sqrt{\pi/|A|}. \text{Note that the Fermi energy \( E_F \) appears in the integration limits defined in Eq. (11).}
\]

while the carrier density \( n \), which is itself a function of \( E_F \), enters explicitly in the self consistent equation for \( V \) [see Eq. (23)]. The cylindrical symmetry around \( K \) and \( K' \) for the dispersion relation in the 4-band model enables the derivation of an analytical expression relating \( E_F \) and \( n \), which reads

\[
E_{F}(n) = \text{sgn}(n) \times \left\{ \begin{array}{ll}
\frac{1}{2} \sqrt{\left( \frac{\pi v_{F}^{2} h^{2} n}{2} \right)^{2} + \xi^{2} + V^{2}} & |n| < \frac{V^{2}}{\pi v_{F}^{2} h^{2}} \\
\sqrt{\pi v_{F}^{2} h^{2} |n| + \xi^{2} + V^{2} - \xi} & \frac{V^{2}}{\pi v_{F}^{2} h^{2}} < |n| < \frac{2V^{2} + V^{2}}{\pi v_{F}^{2} h^{2}} \\
\frac{1}{2} \sqrt{2\pi v_{F}^{2} h^{2} |n| - V^{2}} & |n| > \frac{2V^{2} + V^{2}}{\pi v_{F}^{2} h^{2}} \end{array} \right.
\]

with \( \xi^{2} = t_{\perp}^{2} + (t_{\perp}^{2} + V^{2})\pi v_{F}^{2} h^{2} |n| \). As regards the gap \( \Delta_{q} \), in the 4-band model it is still given by Eq. (23).

For the 2-band model case, the charge imbalance can be written as an integral in momentum space of the function \( |\phi_{B1} - |\phi_{A2}|^{2} = \pm V/(V^{2} + 4v_{F}^{4} p^{4} t_{\perp}^{2})^{1/2} \), where \( \Phi = (\phi_{B1}, \phi_{A2}) \) is the two component wave function obtained by diagonalizing Eq. (11). The \( \pm \) signs stand for the contribution of valence and conduction bands, respectively. In particular, at half-filling the charge imbalance
is given by

$$\Delta n_{1/2} = -\frac{2}{\pi \hbar^2} \int_0^V \frac{d\rho}{\sqrt{V^2 + 4\rho^2 \hbar^2}}$$

$$\simeq -\frac{2}{\pi \hbar^2} \int_0^{2t_\perp} \frac{d\rho}{\sqrt{V^2 + 4\rho^2 \hbar^2}}$$

$$= -\frac{t_\perp V}{2\pi \hbar^2} \ln(2t_\perp /|V| + \sqrt{4t_\perp^2 /V^2 + 1})$$

where we have included a factor of 4 to account for both spin and valley degeneracies. The BZ cutoff $\Lambda$ has been chosen such that $\sqrt{\hbar^2 /m_e} = t_\perp$. This means that the valence and conduction bands are cut off at $\pm(V^2/4 + t_\perp^2)^{1/2}$, exactly the bottom and the top of the highest and the lowest energy bands, respectively, in the 4-band model. This can be justified since for $\nu \rho / \pi \approx t_\perp$ the integrand is of the order $\sim V/t_\perp$, and in the 2-band model it is assumed that $V < t_\perp$. This last inequality enables us to write $\Delta n_{1/2} \approx -t_\perp V/(2\pi \hbar^2) \ln(t_\perp /|V|)$, which, from Eq. (43), leads to the logarithmic divergence of the screening ratio at small external electric field, $E_{\text{ext}}/E \sim -\ln E$, as mentioned in Ref. [88]. For a general filling $n$ the charge imbalance reads

$$\Delta n \approx \frac{t_\perp V}{2\pi \hbar^2} \times$$

$$\left[ -\ln \left( \frac{4t_\perp}{|V|} \right) + \ln \left( \frac{4t_\perp^2 \pi}{t_\perp |V|} + \frac{4\pi^2 \hbar^4 n^2}{t_\perp^2 V^2} + 1 \right) \right]$$

(44)

where the charge density is given in terms of the Fermi wave vector as $n = \pm \rho / \hbar^2$. Inserting Eq. (44) into Eq. (45) we get the following expression for $V$ in the 2-band approximation,

$$V = \frac{n_0 e^2}{2 \pi \hbar^2} d \left\{ \frac{n}{n_0} - 2 + \frac{t_\perp V}{2\pi \hbar^2 n_0} \times$$

$$\left[ -\ln \left( \frac{4t_\perp}{|V|} \right) + \ln \left( \frac{4t_\perp^2 \pi n}{t_\perp |V|} + \frac{4\pi^2 \hbar^4 n^2}{t_\perp^2 V^2} + 1 \right) \right] \right\}$$

(45)

Note that in the 2-band model the gap is exactly the electrostatic energy difference between layers, $\Delta_g = |V|$. In Fig. 6(a) the obtained electrostatic energy difference between planes $V$ is shown for the three different approaches discussed above. The full (black) lines stand for the full tight-binding result, with $V$ given by Eq. (39) and the charge imbalance $\Delta n$ by Eq. (38). The result obtained in the 4-band approximation is shown as dashed (red) lines. It can hardly be distinguished from the full tight-binding result, even when the chemical doping $n_0$ is as high as $5.4 \times 10^{12}\text{cm}^{-2}$ (see figure caption). In fact, the only prerequisite for the continuum 4-band approximation [Eq. (16)] to hold is that $|E_F| << t$, which is always realized for the available BLG devices. As regards the 2-band approximation model, we show as dotted (blue) lines the self-consistent result for $V$, obtained through Eq. (45). Clearly, it is only when both the bilayer density $n$ and the chemical doping $n_0$ are small enough for the relation $|E_F| \ll t_\perp$ to hold that the 2-band model is a good approximation (see inset). The same conclusions apply to the behavior of the gap $\Delta_g$ as a function of carrier density $n$, which is shown in panels 6(b)-(d) for $n_0 = \{0, 1.8, 5.4\} \times 10^{12}\text{cm}^{-2}$, respectively. The failure of the 2-band model in the presence of interactions was also observed in Hartree calculations of the electron compressibility [81].

4. Electron-hole asymmetry

As we have seen in Secs. III.C.1 and III.C.2 the two biased BLG devices shown in Fig. 6(a) have zero gap when the carrier density is twice the system’s chemical doping. The closing of the gap at a finite density induces an electron-hole asymmetric behavior in the system, where obvious examples are the gap $\Delta_g$ and the electrostatic energy difference between layers $V$, as shown in Figs. 6(d) and 6(a). An experimental confirmation for this electron-hole asymmetric behavior comes from measurements of the cyclotron mass in the biased BLG device shown in the left panel of Fig. 6(a) [35] (discussed in more detail in Sec. 6.3). However, real electron-hole asymmetry can also be present in BLG due to extra hopping terms, as mentioned in Sec. III. Here we study how $\Delta_g$ and $V$ are affected by the electron-hole symmetry breaking terms $t’$, $\gamma_4$, and $\Delta$, taking into account the screening correction.

The in-plane second-NN hopping $t’$ gives rise to an
additional term in the Hamiltonian [Eq. (3)] given by

\[ H_{t'} = \sum_{\mathbf{R}, i, \sigma} \sum_{\delta} \left[ a_{i, \sigma}^{\dagger} (\mathbf{R}) a_{i, \sigma} (\mathbf{R} + \delta) + b_{i, \sigma}^{\dagger} (\mathbf{R}) b_{i, \sigma} (\mathbf{R} + \delta) \right], \]

where \( H_{t'} \) is given by Eq. (4), the single layer dispersion \( \epsilon_k \) is given by Eq. (2), and \( \mathbf{1} \) is the \( 4 \times 4 \) identity matrix. An immediate consequence of Eq. (46) is that the BLG dispersion, either biased or unbiased, is given by the \( t' = 0 \) result added by \(-\epsilon^2_{k} t'/t + 3t'\), which clearly breaks electron-hole symmetry. Another consequence is that the presence of a finite \( t' \) has no influence on the wavefunctions’ amplitude. Therefore, the integrand in Eq. (47) – the definition of the charge carrier imbalance between layers \( \Delta n \) – is independent of \( t' \). We have found numerically, using a 4-band continuum model for Eq. (46), that neither the screened \( V \) nor the gap \( \Delta_n \) are affected by \( t' \), although the gap becomes indirect for finite \( t' \). This means that the structure of occupied \( k \)’s is insensitive to \( t' \), and thus \( \Delta_n \) in Eq. (47) is fully \( t' \) independent, at least as long as \( E_F \ll t' \). Even though the presence of \( t' \) can lead to the suppression of the Mexican hat in the valence band, this only happens for \( |V| < t^2 \), \( t' \sim 10^{-3}t \), as can be seen from Eq. (46). For such a small \( |V| \) value the Mexican hat plays an irrelevant role. The band structure around the \( K \) point for \( t' = 0.1t \) (solid line) and \( t' = 0 \) (dashed line) can be seen in Fig. 7(a) for typical parameter values. Now we turn to the effect of the inter-layer second-NN hopping \( \gamma_4 \). This hopping parameter connects equal sublattices \((A1 - A2 \text{ and } B1 - B2)\), and can be taken into account by including the following term in the Hamiltonian [Eq. (3)]:

\[ H_{\gamma_4} = \sum_{\mathbf{R}, \sigma = a, b} \sum_{\gamma} \left[ c_{1, \sigma}^{\dagger} (\mathbf{R}) c_{2, \sigma} (\mathbf{R}) + c_{1, \sigma}^{\dagger} (\mathbf{R} + \mathbf{a}_1) c_{2, \sigma} (\mathbf{R} + \mathbf{a}_2) + h.c. \right]. \]

The generalized version of Eq. (7) now reads

\[ H_{k, \gamma_4} = \begin{pmatrix} V/2 & -t_{\perp} & \gamma_{4} s_{k} & -t_{\perp} \\ -t_{\perp} & V/2 & 0 & \gamma_{4} s_{k} \\ \gamma_{4} s_{k} & 0 & -V/2 & -t_{\perp} \\ -t_{\perp} & \gamma_{4} s_{k} & -t_{\perp} & -V/2 \end{pmatrix}, \]

where \( s_{k} \) is given by Eq. (5). The eigenproblem associated with Eq. (49) admits an analytic treatment at low energies and small biases \( v_F p, V \ll t_\perp \) but as has been seen previously \( V \sim t_\perp \) is possible in real systems. Therefore, we analyze the problem numerically using a 4-band continuum approximation. Equation (49) may then be written as \( H_{k, \gamma_4} = M^T \tilde{H}_{k, \gamma_4} M \) near the \( K \) points, with \( M = \text{diag}[1, e^{i\phi\sqrt{p}}, e^{-i\phi\sqrt{p}}, 1] \) and \( \tilde{H}_{k, \gamma_4} \) given by

\[ \tilde{H}_{k, \gamma_4} = \begin{pmatrix} V/2 & v_F p & -v_F p & -t_{\perp} \\ v_F p & V/2 & 0 & -v_F p \\ -v_F p & 0 & -V/2 & v_F p \\ -t_{\perp} & -v_F p & v_F p & -V/2 \end{pmatrix}, \]

where \( v_F = \gamma_4 a \hbar^{-1} \sqrt{3}/2 \lesssim 10^5 \text{m/s} \). The canonical transformation defined by \( M \) clearly shows that the problem still has cylindrical symmetry in the continuum approximation. Around the \( K' \) points we have \( H_{k', \gamma_4} = M \tilde{H}_{k, \gamma_4} M^T \). The obtained band structure for \( \gamma_4 = 0.1t \) (solid lines) and \( \gamma_4 = 0 \) (dashed lines) is shown in Fig. 7(b) for typical parameter values. Note that, even though the gap becomes indirect for \( \gamma_4 \neq 0 \), we still have \( E_{\pm 0} = \{ \pm V/2, \pm \sqrt{t^2 + V^2/4} \} \) as in the \( \gamma_4 = 0 \) case. The screened electrostatic energy difference between layers \( V \) for the biased BLG device shown in the left panel of Fig. 7(a) is shown as a function of the carrier density in Fig. 7(c). The result for \( V \) has been obtained by solving Eq. (50) with carrier imbalance \( \Delta n \) given by the continuum version of Eq. (47), with wavefunctions obtained numerically through Eq. (50) for \( \gamma_4 = 0.1t \) (see figure caption for other parameter values). The corresponding screened gap \( \Delta_n \) is shown in panel 7(d). The \( \Delta_n = 0 \) result is also shown as a dashed line for both \( V \) and \( \Delta_n \). The effect of \( \gamma_4 \) may clearly be considered small, even for such a large value as \( \gamma_4 \approx 0.3eV \). However, electronic properties which are particularly sensitive to the
changes of the Fermi surface (like, for instance, the cyclotron mass), may, in principle, be measurably affected by $\gamma_4$. We will come back to this point in Sec. 4.

As regards the on-site energy $\Delta$, we can account for it by adding to the Hamiltonian in Eq. 4 the term

$$H_{\Delta} = \Delta \sum_{R, \sigma} \left[ a_{1, \sigma}(R)a_{1, \sigma}(R) + b_{2, \sigma}(R)b_{2, \sigma}(R) \right],$$

(51)

which acts only on sites connected through $t_{\perp}$. Since $\Delta$ is smaller than $\gamma_4$ (see Sec. 4), we consider their simultaneous effect. The term $H_{\Delta}$ adds to $E_{\Delta}$ the contribution $\text{diag}[\Delta, 0, 0, \Delta]$, and therefore the 4-band continuum approximation for finite $\gamma_4$ and $\Delta$ reads

$$\hat{H}_{K, \gamma_4, \Delta} = \begin{pmatrix} V/2 + \Delta & \nu p & -\nu p & -t_{\perp} \\ \nu p & V/2 & 0 & -\nu p \\ -\nu p & 0 & -V/2 & \nu p \\ -t_{\perp} & -\nu p & \nu p & -V/2 + \Delta \end{pmatrix},$$

(52)

where we have applied the same transformation $M$ that lead us to Eq. (22), $H_{K, \gamma_4, \Delta} = M \hat{H}_{K, \gamma_4, \Delta} M$. As previously, the analogues of Eq. (22) near $K'$ is given by $H_{K', \gamma_4, \Delta} = M \hat{H}_{K, \gamma_4, \Delta} M'$, and cylindrical symmetry around $K$ and $K'$ remains. The obtained band structure is shown as solid lines in Fig. 3(a) for $\Delta = 0.01t$ and (b) for $\Delta = -0.01t$, with $\gamma_4 = 0.1t$ and typical parameter values. The dashed lines are the results for $\Delta = 0$ shown in Fig. 3(b). Note that for $p = 0$ the low-energy states are still at $\pm V/2$, while high-energy states are shifted by $\Delta$: $E_{p=0} = \{ \pm V/2, \pm \sqrt{V^2/4 + V^2/4 + \Delta} \}$. Figures 3(c) and 3(d) are the analogous of Figs. 3(c) and 3(d) for finite $\Delta$. Solid lines are the results for $\Delta = 0.01t$ and dotted lines stand for $\Delta = -0.01t$ (see figure caption for other parameter values). The dashed line is the $\Delta = 0$ result. Needless to say, the effect of $\Delta$ is negligible in both $V$ and $\gamma_4$.

D. DOS and LDOS

Insight into the electronic properties of biased (and unbiased) BLG can also be achieved by studying the density of states (DOS) and the local DOS (LDOS) of the system. In particular, the LDOS can be accessed through scanning tunneling microscopy/spectroscopy measurements[22] providing a useful way to validate theoretical models. On the other hand, the knowledge of the DOS turns out to be very useful for practical purposes, as it provides a way to relate the Fermi energy $E_F$ and the carrier density $n$ in the system: $|n| = \int_0^{E_F} dE \rho_2(E)$, where $\rho_2(E)$ stands for the BLG DOS.

We have computed the analytical expression for the DOS of BLG, valid over the entire energy spectrum and for zero and finite bias. The expression is given in Appendix D. As regards the LDOS, the results have been obtained using the recursive Green’s function method[23]. The DOS and LDOS of unbiased BLG has been obtained previously within the effective mass approximation in Ref. 4. The effect of disorder on the DOS and LDOS of BLG, both biased and unbiased, has also been studied recently[41,50,51,52,84,85].

The unbiased LDOS for sites that connect the two layers through $t_{\perp}$, i.e. $A1$ and $B2$, and sites disconnected from the other layer, i.e. $B1$ and $A2$, is shown in the left inset of Fig. 3(a) along with the total unbiased DOS. Although the DOS of BLG is finite at zero energy, the LDOS at $A1$ and $B2$ sites vanishes linearly when $E \rightarrow 0$. The finite contribution to the DOS comes from the LDOS at sites that are disconnected from the other layer, $B1$ and $A2$. This is due to the nature of the zero energy states at the Dirac points in BLG. As can be seen in Eq. (23), these quasiparticles have finite amplitude only in the $B1$ and $A2$ sublattices, which are not coupled. Note that this asymmetry between sublattices belonging to the same layer plays a central role in the 2-band continuum model given in Eq. (11), where only $B1$ and $A2$ sites are taken into account in determining the low energy behavior. This scenario has been confirmed experimentally through STM measurements[48,61], where the full hexagonal symmetry of the honeycomb lattice appears as a reduced threefold symmetry, characteristic of a triangular lattice, in agreement with the abovementioned low energy description.

As for the DOS in the presence of a finite bias the following values for $\alpha(V, t_{\perp}) = (V^4/4 + t_{\perp}^2 V^2/2)/(V^2 + t_{\perp}^2)$ are shown in Fig. 4(a): $\alpha = 10^{-4}$, $10^{-3}$, and $10^{-2}$ ($V \approx 0.014t$, $0.045t$, and $0.14t$, respectively, for $t_{\perp} = 0.2t$). The 1D-like divergence (right inset) seen at the minimum of the low-energy bands $|E_k^\pm|$ occurs as long as the solution of Eq. (20) exists, i.e., for $\alpha(V, t_{\perp})$ in

\[ \Delta = 0.01t \]

\[ \Delta = -0.01t \]

\[ V_{\text{bias}}(V,t) \]

\[ n(V,t) \]

\[ \Delta_g \]

FIG. 8: (Color online) (a)-(b) Band structure around the $K$ point for the biased BLG with $\Delta = 0.01t$ and $\Delta = -0.01t$, respectively, for $V = t_{\perp} = \gamma_4 = 0.1t$. Dashed lines stand for $\Delta = 0$. (c)-(d) Respectively, screened $V$ vs $n$ and $\Delta_g$ vs $n$ for the biased BLG device shown in the left panel of Fig. 3(a), modeled with a finite $\Delta$: solid lines for $\Delta = 0.01t$ and dotted lines for $\Delta = -0.01t$. Parameters: $t \approx 3eV$, $t_{\perp} = 0.1t$, $\gamma_4 = 0.1t$, $\epsilon_r = 1$, and $n_0 = \{0,1.8\} \times 10^{12} \text{cm}^{-2}$. Dashed lines stand for $\Delta = 0$.0.
as \( \rho_{B1/A2}(E) = \frac{1}{\sqrt{2\pi}} \sum_k |\phi_{B1/A2,k}|^2 \delta(E - E_k) \), where \( \phi_k = (\phi_{B1,k}, \phi_{A2,k}) \) is the two component wave function obtained by diagonalizing Eq. (11), we can readily arrive at the following expressions,

\[
\rho_{B1/A2}(E) = \frac{1}{2\sqrt{3\pi}} t_\perp \text{sign}(E) \frac{E \pm \sqrt{V^2/4 - E^2}}{\sqrt{V^2/4 - E^2}}.
\]  

The asymmetric behavior is apparent, with \( \rho_{B1}(E) \) diverging for \( E \to V/2^+ \) and \( \rho_{A2}(E) \) for \( E \to -V/2^- \). The result for \( \rho_{A2}(E) \) is shown in Fig. 4(d) for \( V \approx \{0.87, 4.23, 7.87\} \times 10^{-3}\) and \( t_\perp = 0.1t \). Within the screening corrected parallel plate capacitor model discussed in Sec. III (Eq. 39), these \( V \) values correspond to carrier densities \( n \approx \{0.2, 0.8, 1.4\} \times 10^{12}\) cm\(^{-2}\), respectively, where we have used \( t \approx 3.1\) eV, \( n_0 = 0 \), and \( \varepsilon_r = 1 \). The full lines are the recursive Green’s function method results and dashed lines are the results of Eq. (33). As expected, the closer to the gap edges the better the agreement between the two approaches.

A strong suppression of electrical noise in BLG has been reported recently by Lin and Avouris.\(^{32}\) In devices made from exfoliated BLG on top of SiO\(_2\), the current fluctuations are thought to originate from the fluctuating trapped charges in the oxide. Therefore, the more effective the impurity charge screening in the system the lower the electrical noise. The lower noise in BLG than in SLG may then be attributed to the low energy finite DOS in the former. However, it has also been reported in Ref. 32 that while increasing the carrier density \( n \) in SLG leads to lower noise, as expected due to more effective impurity screening, it results in higher noise in BLG. Insight into this behavior is achieved by analyzing the LDOS at the Fermi level \( E_F \) in a biased BLG, as charging the system through the back gate \( V_g \) leads to a finite perpendicular electric field. In Fig. 9(c) we show the biased BLG LDOS at \( E_F \) for \( B1 \) and \( A2 \) sites as a function of carrier density \( n \) in the system. For a given \( n \), the electrostatic energy difference \( V \) is evaluated self-consistently through Eq. (33), with \( n_0 = 0 \) and \( \varepsilon_r = 1 \), and \( E_F \) is obtained by integrating over the DOS. Additionally, we use \( t \approx 3\) eV and \( t_\perp = 0.1t \). We have chosen densities in the range \( n \in [0 - 2] \times 10^{12}\) cm\(^{-2}\), which corresponds to back gate voltages \( \Delta V \approx [0 - 27] \) eV through Eq. (43), similar to the experimental range in Ref. 32. The main observation to be made as regards the results of Fig. 9(c) is that for the low energy active sublattices \( B1 \) and \( A2 \) the LDOS at \( E_F \) remains approximately constant with increasing electron density \( n \), as opposed to the \( \sim \sqrt{n} \) dependence found in SLG. This is an indication that impurity screening may not be increasing with carrier density in the biased BLG system, which may be contributing to enhance electrical noise.

### IV. MAGNETIC FIELD EFFECTS

As mentioned in Sec. I, both the SLG and the unbiased BLG show anomalous integer QHE’s, which provides a
clear feature of the unusual electronic properties in these systems. In SLG, the Hall conductivity $\sigma_{xy}$ was shown to be characterized by an anomalous integer quantization rule $^{11,12}$

$$\sigma_{xy} = \pm \frac{4e^2}{h} \left( n + \frac{1}{2} \right), \quad n = 0, 1, 2, \ldots \quad (54)$$

where the $\pm$ signs stand for electron and hole-like carrier types, while in BLG there is a distinct double step at the neutrality point $^{13}$ when charge carriers change type,

$$\sigma_{xy} = \pm \frac{4e^2}{h} (n + 1), \quad n = 0, 1, 2, \ldots \quad (55)$$

For the biased BLG, as a consequence of the gapped band structure discussed in Sec. III, a perpendicular magnetic field is expected to induce distinct features in electronic properties, and ultimately lead to a different quantization rule for the Hall conductivity. In this section we focus on the semi-classical approach to the cyclotron mass, Landau level quantization and related integer QHE.

A. Cyclotron mass

In the semi-classical approximation the cyclotron effective mass $m_c$ is given by

$$m_c = \frac{\hbar^2}{2\pi} \left( \frac{\partial A(E)}{\partial E} \right)_{E=E_F}, \quad (56)$$

where $A(E)$ is the $k$-space area enclosed by the orbit of energy $E$, and the derivative is evaluated at the Fermi energy $E_F$. \textsuperscript{26,90,91} It can be accessed experimentally through the Shubnikov-de Haas effect, providing a direct probe to the Fermi surface. In the case of exfoliated graphene, either SLG or (un)biased BLG, the Fermi energy can be varied by tuning the back gate voltage, and therefore a significant portion of the whole band structure may be unveiled. In particular for the biased BLG, the presence of a finite gap can be checked and the model developed in Sec. III tested.

1. Comparison with experiment

General expressions for $m_c$ obtained for the full tight-binding bands in Eq. (19), valid for the relevant parameter range $V \lesssim t_{\perp} \ll t$ and restricted to $E_F < t$, are given in Appendix C. In Fig. 10(a) we compare the theory results for the cyclotron mass with experimental measurements\textsuperscript{26} on the biased BLG system shown in the left panel of Fig. 3(a). We have only considered $m_c$ associated with low energy bands $E_{k}^{-}$ [see Eq. (19)], since $E_{k}^{\pm}$ are inactive for the experimentally available carrier densities. The dashed lines stand for the unscreened result, where $V$ is given by Eq. (34), and the solid lines are the screened result, with $V$ given by Eq. (29). The inter-layer coupling $t_{\perp}$ has been taken as an adjustable parameter, keeping all other fixed: $t \simeq 3eV$, $\varepsilon_{r} = 1$, and $n_{0} = 1.8 \times 10^{12} cm^{-2}$. The value of $t_{\perp}$ could then be chosen so that theory and experiment gave the same $m_c$ for $n = 2n_{0} \approx 3.6 \times 10^{12} cm^{-2}$. As discussed in Sec. IIIC2 at this particular density the gap closes, meaning that the theoretical value becomes independent of the screening assumptions. We found $t_{\perp} \simeq 0.22 eV$, in good agreement with values found in the literature. The theoretical dependence $m_c(n)$ agrees well with the experimental data for the case of electron doping. Also, as seen in Fig. 10(a), the screened result provides a somewhat better fit than the unscreened model, especially at low electron densities. This fact, along with the good agreement found for the electrostatic energy difference data of Ref. 33 [see Fig. 6(c)], allows us to conclude that for doping of the same sign from both sides of bilayer graphene, the gap is well described by the screened approach. In the hole doping region in Fig 10(a), the Hartree approach underestimates the value of $m_c$ whereas the simple unscreened result overestimates it. This can be attributed to the fact that the Hartree theory used here is reliable only if the gap is small compared to $t_{\perp}$. In the experimental realization of Ref. 33 $n_{0} > 0$ and, therefore, the theory works well for a wide range of electron doping $n > 0$, whereas even a modest overall hole doping $n < 0$ corresponds to a significant electrostatic difference between the two graphene layers. In this case, the unscreened theory overestimates the gap whereas the Hartree calculation underestimates it. However, it is clear that the experimental data in Fig 10(a) interpolate between the screened result at low hole doping and the unscreened one for high hole densities. This indicates that the true gap actually lies between the unscreened and screened limits [see Fig. 5(d)], and that a more accurate treatment of screening is needed when $V$ becomes of the order of $t_{\perp}$.

In Fig 10(b) we compare our best fit to the cyclotron mass (full line) with results obtained for different param-
eter values. The dashed-dotted lines stand for \( m_e \) obtained with \( \varepsilon_r = 2 \) in Eq. 59. As can be seen clearly, the \( n > 0 \) result is not substantially affected, while for \( n < 0 \) the theory description of \( m_e \) worsens. This is due to the reduction of the gap when \( \varepsilon_r \) is increased [see left inset in Fig. 5(d)]. The dashed lines in Fig. 10(b) are obtained with \( n_0 = 0 \), where the zero gap occurs at the neutrality point. The dotted lines are the result for \( \varepsilon_{ext} = 0 = V \), i.e., zero gap at every density value. Note that these two results, \( n_0 = 0 \) and \( V = 0 \), show an electron-hole symmetric \( m_e \), contradicting the experimental result. It may then be said that the electron-hole asymmetry observed in \( m_e \) is a clear indication of the presence of a finite gap in the spectrum. It will be shown in Sec. 1V.A.3 that, if we ignore the gap, this electron-hole asymmetry cannot be described by taken into account \( t' \) or \( \gamma_4 \).

2. Cyclotron mass in continuum models

Here we compare our results for the cyclotron mass, which has been obtained with expressions shown in Appendix C with the results of continuum models.

Within the 4-band continuum model given by Eq. 10, where the dispersion is just the full tight-binding result [Eq. 19] with the substitution \( \varepsilon_k \rightarrow \omega \), we can easily derive the following analytical expression for \( m_e \),

\[
m_e = \frac{E_F}{\omega_F} \left[ 1 + \frac{V^2 + t_1^2}{2E_F^2(V^2 + t_1^2) - t_1^2V^2/4} \right].
\]

In Fig. 11(a) the dashed line is the result of Eq. 57, where \( V \) has been computed self-consistently using Eq. 39 and the 4-band continuum approximation discussed in Sec. 1V.C.3. As expected, the agreement with the full tight-binding result (shown as a full line) is excellent for the considered densities. Note that there is an extra solution given by \( m_{e,1}^\text{extra} = E_F \{1 - (V^2 + t_1^2)/\sqrt{4E_F^2(V^2 + t_1^2) - t_1^2V^2} \} \), valid when \( |E_F| < V/2 \) or \( |E_F| > \sqrt{V^2/4 + t_1^2} \), which corresponds to the extra orbit appearing when \( E_F \) falls in the Mexican-hat region, or above the bottom of high energy bands. With \( E_F \) given by Eq. 12, we can readily estimate the densities for which these two regions start playing a role. Using \( V \sim 0.1t_\perp \sim 0.01t \) in the Mexican hat region (valid for \( n_0 \leq 2 \times 10^{12} \text{cm}^{-2} \)) we get \( n \leq 10^{11} \text{cm}^{-2} \); setting \( V \sim t_\perp \sim 0.1t \) around the bottom of high energy bands we get \( n \geq 10^{13} \text{cm}^{-2} \). These two density values are outside the range of experimentally realized densities [see Fig. 10(a)].

The continuum approximation can be used to better understand the behavior of \( m_e \). At very low densities and not so high external electric field, say \( E_F \ll V \ll t_\perp \), we may use the Mexican hat dispersion given in Eq. 21. Taking into account the cylindrical symmetry around \( K \) and \( K' \), we obtain for the cyclotron effective mass

\[
m_e \approx \frac{Vt_\perp^2}{2\pi\hbar^2\omega_F} \frac{1}{|n|}.
\]

which explains the the \( n^{-1} \) divergence at low densities. This result is exactly the same obtained inserting Eq. 12 for \( |n| < \bar{n} = V^2/(4\pi^2\hbar^2) \) into Eq. 57, and taking the limit \( |n| \ll \bar{n} \). It should be noted, however, that at very low densities the semi-classical approximation fails: the correspondence principle is not expected to be valid when only few Landau levels are occupied.

As shown in Ref. 10, the cyclotron mass for the unbiased BLG in the continuum approximation is given by

\[
m_e = m^* \sqrt{1 + 4\pi\hbar^2\omega_F^2/n|t_\perp|^2},
\]

where \( m^* = m_e(0) = t_\perp/(2\omega_F^2) \sim 3 \times 10^{-2}m_e \) is the effective carrier mass at low densities for the unbiased BLG. This equation may be obtained through the dispersion given in Eq. 12, or by setting \( V = 0 \) in Eq. 57 and using the appropriate relation \( E_F(n) \) from Eq. 12. This explains the behavior \( \sqrt{|\text{const} + n|} \) as the density is increased, shown in Fig. 10(b).

3. Effect of electron-hole asymmetry

In Sec. 1V.C.3 the effect of electron-hole symmetry breaking parameters - namely, \( t' \), \( \gamma_4 \), and \( \Delta \) - has been studied regarding the self-consistent description of the gap. Here we extend the analysis to the cyclotron mass, restricting ourselves to the biased BLG device shown in the left panel of Fig. 4(a).

Results for finite \( t' \), \( \gamma_4 \), and \( \Delta \), have been obtained within the 4-band approximation model. As all cases have cylindrical symmetry around \( K \) and \( K' \), the cyclotron mass may be written as \( m_e = \omega_F/(\partial E_F/\partial \omega_F) \).

For finite \( t' \) it is possible to derive an analytical expression for \( m_e \) in terms of the Fermi momentum \( \omega_F \). However, the relation between \( \omega_F \) and the Fermi energy \( E_F \) is determined numerically through the continuum version of Eq. 12. For finite \( \gamma_4 \) and \( \Delta \) the calculation is fully numerical, based in Eqs. 50 and 52.

In Fig. 11(b) we show the \( m_e \) result for finite \( t' \) (dotted red line) and finite \( \gamma_4 \) (dashed blue line), keeping \( n_0 = 0 \) (absence of electron-hole asymmetry due to chemical doping). The thin full line is the result obtained for \( t' = \gamma_4 = 0 \) in Sec. 1V.A.1 and circles are experimental data from Ref. 33. The \( n > 0 \) region, where the smaller gaps are realized experimentally, is still well fitted if we choose \( t_\perp \approx 0.022eV \) with \( t' \approx 0.3eV \) or \( t_\perp \approx 0.19eV \) with \( \gamma_4 \approx 0.12eV \) (we use \( t \approx 3eV \)). However, it is clear that neither of these results can account for the electron-hole asymmetry observed experimentally. In fact, a closer look reveals that the \( m_e \) for finite \( t' \) have the opposite trend, being smaller than the \( t' = 0 \) result for \( n < 0 \) and larger for \( n > 0 \), as would be expected by inspection of the energy bands in Fig. 4(a). Such an opposite trend should also be seen for finite \( \gamma_4 \), although the effect is not as large as expected from the considerable distortion of the energy bands shown in Fig. 11(b). This attenuation can be understood as the result of fixing the carrier.
density $n$ and not the Fermi energy $E_F$: changing $\gamma_4$ (or $t'$) for a given $n$ leads to a different $E_F$, and the new $E_F$ is such that it counteracts the expected effect of $\gamma_4$ (or $t'$) in $m_c$. Fig. 11(c) shows the same as 11(b) for $n_0 = 1.8 \times 10^{12} \text{cm}^{-2}$. The effect of the on-site energy $\Delta$ is shown in Fig. 11(d) for fixed $\gamma_4 \approx 0.12 \text{eV}$, $\nu_1 \approx 0.19 \text{eV}$ and $n_0 = 1.8 \times 10^{12} \text{cm}^{-2}$. The result for $\Delta = 0$ (dashed line) is shown along with the result for $\Delta \approx 0.03 \text{eV}$ (full line) and $\Delta \approx -0.03 \text{eV}$ (dotted-dashed line). It is clear that the effect of $t'$, $\gamma_4$ and $\Delta$ on the cyclotron mass can be neglected.

B. Landau level quantization and QHE

In this section we consider the full quantum mechanical problem of a (un)biased BLG subjected to a perpendicular magnetic field. The presence of a perpendicular magnetic field $B = B_0 \hat{z}$ is accounted for through the standard Peierls substitution,$^{70,71,72,73}$ $t \rightarrow t \exp \{ i e \cdot R \cdot \delta \cdot \hat{A} \}$, where $e$ is the electron charge, $\delta$ the vector connecting NN sites, and $\hat{A}$ the vector potential (in units such that $c = 1 = \hbar$). The BLG tight-binding Hamiltonian may still be written as in Eq. 6 with the SLG terms $H_i$

rewritten as

$$H_i = -t \sum_{\mathbf{R},\sigma} \left[ e^{-i \varphi_i(R)} a_{i,\sigma}^\dagger(R) b_{i,\sigma}(R) + e^{i \varphi_i(R)} a_{i,\sigma}^\dagger(R) b_{i,\sigma}(R - a_1) + a_{i,\sigma}^\dagger(R) b_{i,\sigma}(R - a_2) + \text{h.c.} \right]$$

where $\varphi_i(R) = [R \cdot \hat{a}_i^2/(a \sqrt{3}) + \delta_{2}/2] \phi/\phi_0$. The Peierls phase in Eq. (60) is written assuming a Landau gauge, $\mathbf{A} = (-y, 0, 0) B$, where $\phi/\phi_0 = B A_0/\phi_0$ is the magnetic flux through a plaquette in units of the flux quantum $\phi_0 = h/e$ ($A_0$ being the area of the graphene unit cell). Note, however, that the minimum plaquette for bilayer graphene is one third of the hexagonal unit cell (dashed area on the right panel of Fig. 11), where the magnetic flux is $\phi/3$.

The effect of a perpendicular magnetic field can also be studied within the continuum approximation through minimal coupling $p \rightarrow p - e \mathbf{A}$. The case of biased BLG has been studied both within the 4-band [Eq. (10)] and 2-band [Eq. (11)] continuum models in Refs. 50, 51, 52, 53. Here we present results obtained with the full tight-binding model given by Eqs. 5 and 60. The problem is treated numerically for finite width ribbons, with the obvious advantage that we can analyze the differences between zigzag and armchair edges, and study how the magnetic field affects surface states in zigzag edges.$^{62}$ The unbiased BLG with zigzag edges has been studied recently for rational flux $\phi = p/q$. When a rational flux is considered in Eq. (20), we may again impose periodic boundary conditions according to the magnetic translation sub-group, and find the usual Hofstadter butterfly.$^{63}$ That has recently been done for the unbiased BLG.$^{64}$

1. Unbiased bilayer

In the ribbon geometry, translational invariance along the longitudinal direction is preserved by the vector potential field. Hence, we can calculate the band structure using the same quantum number $k$ as in the absence of the magnetic field. The Landau level structure for a BLG ribbon under a 30 T magnetic field (no bias) is shown in Fig. 12(a) for zigzag edges, and 12(b) for armchair edges. Non-zero bulk Landau levels are clearly visible around the Dirac points: $k_{\perp}^2, a = 2\pi /3, 4\pi /3$ for zigzag and $k_{\perp}^2, a = 0$ for armchair edges. As in the case of standard 2D electron gases and SLG, the transversely localized wave functions (Landau states) move across the ribbon as $k$ is increased. As the wave function approaches the edges the energy of electron (hole) Landau levels shifts up (down). For the zigzag ribbon result shown in Fig. 12(a), we can clearly see the zero energy flat bands, which are practically unchanged when compared with the case without magnetic field.$^{65}$ However, these bands are made up of both bulk Landau levels and surface states as in the case of SLG.$^{66,67}$ which becomes apparent in the
presence of the bias (see below). As expected for the armchair ribbon, the zero energy bands shown in Fig. 12(b) are only made up of zero energy bulk Landau levels.

The ribbon geometry mirrors exactly Laughlin’s geometry used in the context of QHE. Laughlin-Halperin’s argument allows us to compute the Hall conductivity from the number of edge states crossing the Fermi level. If the chemical potential is above the nth level there are 2n + 2 edge states per edge crossing the Fermi level. The Hall conductivity, including the spin degeneracy, is then given by Eq. (60). This has been experimentally confirmed. The unusual behavior occurs when the Fermi level crosses the neutrality point, making the Hall conductivity to change from $\sigma_{xy} = -4e^2/h$ to $\sigma_{xy} = 4e^2/h$, giving rise to a double step of $8e^2/h$.

Equivalent conclusions can be reached within the continuum approximation. In the 4-band model standard manipulations lead to the Hamiltonian

$$H_K(n) = \begin{pmatrix} 0 & \gamma \sqrt{n} & 0 & t_\perp \\ \gamma \sqrt{n} & 0 & 0 & 0 \\ 0 & 0 & \gamma \sqrt{n+1} & 0 \\ t_\perp & 0 & \gamma \sqrt{n+1} & 0 \end{pmatrix} \tag{61}$$

for valley $K$, where $\gamma = \sqrt{2/3} l_B/h$, with $l_B = \sqrt{|e|B}/|B|$ for the magnetic length. The Hamiltonian for valley $K'$ can be obtained from Eq. (61) with the substitution $\sqrt{n} \to \sqrt{n+1}$ and $\sqrt{n+1} \to \sqrt{n}$. The Landau level label takes values $n = -1, 0, 1, 2, 3, \ldots$. The resultant Landau level spectrum is given by

$$E_{n}^{\pm} = \pm \sqrt{(1 + 2n) \gamma^2 + \frac{t_\perp^2}{2}} \pm \sqrt{(\gamma^2 + t_\perp^2)^2/4 + n \gamma^2 t_\perp^2}, \tag{62}$$

where non-zero ($n \geq 1$) eigenenergies are fourfold degenerate due to valley and spin degeneracy, while zero energy Landau levels have eightfold degeneracy, since there are two zero energy Landau states ($n = -1, 0$) per valley per spin. This eightfold degeneracy accounts for the double step $8e^2/h$ in the Hall conductivity [Eq. (59)]. The 2-band model result $E_{n}^{\pm} \approx \pm \gamma t_\perp^{-1} \sqrt{n(n+1)}$ is easily recovered from Eq. (62) for $\gamma \ll t_\perp$ being valid for magnetic fields up to $B \approx 1T$.\[^{57}\]

FIG. 12: (Color online) Energy spectrum for an unbiased BLG ribbon with zigzag (a) and armchair (b) edges in the presence of a magnetic field $B = 30T$. The ribbon width was set to $N = 400$ and $t_\perp = 0.2t$.

FIG. 13: (Color online) Energy spectrum for a BLG ribbon with zigzag edges in the presence of a finite bias and magnetic field $B = 30T$: (a)-(d) $V = t_\perp/10, t_\perp/5, t_\perp/2, t_\perp$, respectively. The inter-layer coupling was set to $t_\perp = 0.2t$ and $N = 400$ in all panels.

2. Biased bilayer

When, in addition to a magnetic field, the BLG ribbon is subjected to a bias, the degeneracy of zero energy bands is lifted. Two flat bands with energies $-V/2$ and $V/2$ appear, similarly to the case with no magnetic field. This is clearly seen in Fig. 13a where we show the energy spectrum for a BLG ribbon with zigzag edges in the presence of a finite bias and magnetic field $B = 30T$. The other two zero energy bands become dispersive inside the gap showing the band crossing phenomenon. For $B = 30T$ the Landau level spacing is set by $\gamma$ [Eq. (62)], which is of order of $t_\perp$. Therefore, as long as $V \ll t_\perp$, the bias is much smaller than Landau level spacing. Thus, non-zero energy bulk Landau levels are almost unchanged, as can be seen in Fig. 13(a)-(b), except for a small asymmetry between Dirac points which we discuss below. For larger $V$ values the cyclotron frequency becomes $V$ dependent, decreasing with increasing $V$, as can be seen in Fig. 13(c)-(d). For $V \geq t_\perp$ the dispersive modes start crossing with non-zero bulk Landau levels.

The Landau level transition energies in BLG have been recently obtained through cyclotron resonance measurements. The data was found to deviate from what would be expected through Eq. (62), especially for larger filling factors. It should be noted, however, that in order to keep a constant filling factor and vary the magnetic field, as done in Ref. 100, the back gate voltage $V_g$ has to be tuned to compensate for the variation of Landau level degeneracy. As we have seen previously, tuning $V_g$ is equivalent to change $V$ – the electrostatic energy difference between layers – which means that Eq. (62) is no longer valid, as recently shown within the 4-band continuum model. To have an estimate for the effect of the back gate voltage on the Landau level spacing we have computed Landau level energy differences taking...
into account the variation of $V$ with carrier density $n$. We have used the unscreened result given by Eq. (51), with $n_0 = 0$ and $\varepsilon = 1$. Within this approximation we can easily write $V$ in terms of the filling factor $\nu$ and magnetic field $B$ as $V = \nu B e^2 d/(2\varepsilon_0 \Phi_0) \approx 7.4 \times 10^{-4} \nu B$, with $B$ in Tesla in the last step. Thus, for fixed filling factor, $V$ varies linearly with $B$. Note that the comparison between this unscreened treatment of the biased BLG and the unbiased result in Eq. (52) should give lower and upper limits for the effect of the perpendicular external field in the cyclotron frequency. In Fig. 14 we show the obtained Landau transition energies vs magnetic field for the given filling factors. The dashed lines represent the unbiased BLG result, as given by Eq. (52). The lines with crosses are the results for the unscreened biased BLG, and filled symbols are experimental data from Ref. 100. Circles for $\nu > 0$ and squares for $\nu < 0$. We have used $t = 3.5 eV$ and $t_d = 0.1 t$, consistent with Ref. 100. As can be seen from Fig. 14, the back gate induced electric field gives rise to sizable effects already for magnetic fields and filling factors realized in experiments. Except at $\nu = \pm 8$, the result of Eq. (52) for the unbiased and the unscreened biased BLG result effectively provide upper and lower limits to the experimental data. The observed electron-hole asymmetry could then be interpreted as due to an asymmetry in $V$ vs $n$: larger $V$, and therefore larger gap, for $n < 0$; smaller $V$ and gap for $n > 0$, which would make the result more close to the unbiased case. It should be noted that in such a case we would expect the neutrality point to occur for $V_0 < 0$, as is the case of the NH$_3$ doped BLG studied before. For the system reported in Ref. 100, however, the opposite seems to be happening, as indicated by the Hall resistivity. A neutrality point for $V_0 > 0$ is, in fact, the more usual effect of H$_2$O molecules adsorbed on graphene samples. As a final remark regarding the results presented in Fig. 14 we note that the experimental data trend, which makes Eq. (52) a poor fit at $|\nu| \geq 8$, is still not accounted for in the biased BLG result. An alternative approach is the inclusion of the screening correction, which should go beyond Eq. (55) including the magnetic field effect. It has been reported recently that Dirac liquid renormalization may also be contributing to the observed trend.

We now address the QHE in biased BLG. We have analyzed the character of the eigenstates for the two flat bands at $\pm V/2$ and for the other two bands dispersing inside the gap. The result is shown in Figs. 15 and 16, where the top left panel of 15(a), 15(b), 16(a), and 16(b) show the abovementioned bands and indicates, as vertical dashed lines, the $k$-points for which the wave functions have been computed. Figure 15(a) considers the flat band with energy $V/2$. A left edge state becomes a bulk Landau state living at sublattice $B1$ as the first Dirac point $k \approx 2\pi/3$ is reached. As $k$ is increased this bulk Landau state traverse the sample, transforming into a surface state localized at the right edge of layer 1. The flat band with energy $-V/2$ [Fig. 15(b)], on the other hand, starts with a left surface state living at sublattice $A2$, which becomes a bulk Landau state at the second Dirac point $k \approx 4\pi/3$. Then, the bulk Landau state traverse the sample as $k$ is increased, ending in a right edge state. Figure 16(a) shows the result obtained for the hole-like dispersive band. The portion of the band having energy approximately $V/2$ corresponds to a left surface state localized mainly at sublattice $A1$. At the Dirac point $k \approx 4\pi/3$ it changes layer, becoming a bulk Landau state living at sublattice $A2$ with energy $-V/2$. As regards the electron-like dispersive band in Fig. 16(b), beyond the Dirac point $k \approx 2\pi/3$ the left edge state becomes a bulk Landau state living at sublattice $B1$ with energy around $V/2$. After traversing the sample it changes layer, and transforms into a surface state localized mainly at the right edge of layer 2, sublattice $B$, with energy $-V/2$. The overall situation is summarized in the sketch shown in Fig. 17(a). Full lines stand for bulk Landau states and dashed lines represent edge states. Note that quasi-degeneracies have been removed in order to make the figure clear. The reason for band crossing between dispersive bands becomes apparent in this sketch, as in the crossing region one band corresponds to bulk Landau states and the other to surface states, which do not overlap.

Now imagine that the chemical potential occurs inside the gap, between the last hole and the first electron-like bulk Landau levels, crossing the dispersive bands as shown in Fig. 17(a). As pointed out by Laughlin, changing the magnetic flux through the ribbon loop by a flux quantum makes the states to move rigidly towards one edge of the sample. In the usual integer quantum Hall effect, the energy increase due to this adiabatic flux variation results from the net transfer of $n \times g$ electrons (spin and valley degeneracy $g$) from one edge to the other, and the quantization of the Hall conductivity follows, $I/\nu = gne^2/h$, where $I$ is the current carried around

FIG. 14: (Color online) Landau level transition energies vs magnetic field for the given filling factors. The dashed line is the unbiased BLG result as given by Eq. (52) and the line with crosses is the biased BLG result (see text). We have used $t = 3.5 eV$ and $t_d = 0.1 t$. Filled symbols are experimental data from Ref. 100. Circles for electrons and squares for holes.
the loop and \( V \) the potential drop from one edge to the other. However, in the present case there is no net charge transfer across the ribbon. As seen in Fig. 17(a), the rigidity movement of the states towards one edge makes an electron-hole pair to appear in both edges, resulting in zero net charge transfer. Therefore, the Hall conductivity of the biased bilayer is given by,

\[
\sigma_{xy} = \pm 4n e^2/h, \quad n = 0, 1, 2, \ldots \tag{63}
\]

with a Hall plateau \( \sigma_{xy} = 0 \) showing up when the carriers change from hole to electron-like, i.e., when the doping crosses the zero value. Note that at this particular Hall plateau the current carried around the ribbon loop is zero, \( \mathcal{I} = 0 \), which implies an infinite longitudinal resistivity, \( \rho_{xx} \to \infty \), at odds with standard Hall plateaus. This scenario has been confirmed experimentally.\(^\text{23}\) The same conclusions can be drawn from the armchair BLG ribbon, as shown in Fig. 17(b). In that case the \( \sigma_{xy} = 0 \) plateau follows directly from the opening of a gap.

A close inspection of Fig. 17 shows that the valley degeneracy is in fact lifted, which is also seen for the ribbon with armchair edges [Fig. 17(c)]. This is due to the different nature of the Landau states at valley \( K \) and \( K' \) with respect to their projection in each layer. Actually, the Landau states of the unbiased BLG for valley \( K \) have different weight on layer 1 and layer 2 when compared to their degenerate counterparts at valley \( K'/\perp \). This is equivalent to a small charge imbalance between the layers, with opposite sign in valley \( K \) and \( K' \). When the layers are made inequivalent by the bias, the bulk Landau levels at one valley move downward in energy, whereas those at the other move upward. The energy of the modified Landau levels is given by Hamiltonian \( \mathbf{H}_\parallel \), and its counterpart in valley \( K' \), with the matrix diagonals replaced by \( (V/2, V/2, -V/2, -V/2) \). In the limit of small bias \( V \ll \gamma \) the Landau level energy splitting takes the form

\[
\delta E_n \approx \frac{V}{\sqrt{(1 + \gamma^2/\ell_1^2)^2 + 4n^2\gamma^2/\ell_1'^2\ell_1^2}}. \tag{64}
\]

The valley asymmetry has a stronger effect in the zero energy Landau levels, where the charge imbalance is saturated. This makes a gap \( V \) to open, and leads to the \( \sigma_{xy} = 0 \) Hall plateau. However, there is also an intra-valley degeneracy lifting, as only one of those two Landau states remain an eigenstate of the biased system. This intra-valley energy splitting has exactly the value given
FIG. 16: (Color online) Module square of the wave function for the bands closer to zero energy: (a) dispersive hole like band inside the gap; (b) dispersive electron like band inside the gap. Magnetic field $B = 30$ T, bias $V = t_{\perp}/10$, and $t_{\perp} = 0.2t$ for a BLG ribbon with zigzag edges and $N = 400$.

FIG. 17: (Color online) (a) Sketch of the bands closer to zero energy with indication of bulk or edge character, as well as left or right position, for a BLG ribbon with zigzag edges in the presence of a finite bias and magnetic field. (b) Energy spectrum for a BLG ribbon with armchair edges, for $B = 30$ T, $V = 0.14t_{\perp}$, and $t_{\perp} = 0.2t$.

by Eq. (64) for $n = 0$, to first order in the bias. Therefore, new Hall plateau at half integer values in Eq. (63) may appear as long as the Landau level splitting can be experimentally resolved. As an example, taking $t_{\perp} \approx 0.1t$ and $n = 0$ in Eq. (63), we obtain a Landau level splitting of $\delta E_0 \sim V/10$ for a 10 T magnetic field, raising to $\delta E_0 \sim V/3$ at 35 T.

The electronic spectrum for BLG in a magnetic field is shown in Fig. 18 for a rational flux $\phi/\phi_0 = p/q$. Fig. 18(a) shows the SLG spectrum for comparison, (b) and (c) are the results for unbiased and biased BLG, respectively. It is clear that the spectrum has the recursive structure of the Hofstadter butterfly. Standard symmetries also hold for BLG, namely, translations $\phi \rightarrow \phi + 3n\phi_0$, with $n$ integer, and reflections $E \rightarrow -E$ and $\phi \rightarrow -\phi$ do not change the energy spectrum. The invariance under translations $\phi \rightarrow \phi + n\phi_0$ is present in SLG (51), which, in connection with the $\phi \rightarrow -\phi$ symmetry, implies that the spectrum has the reflection symmetry about $\phi/\phi_0 = 1/2$. In the case of BLG, only translations of flux that are a multiple of $3\phi_0$ map the system back to itself. This has to do with our choice for the hopping phases in the Peierls substitution. As shown in Fig. 11, the magnetic flux through the minimum plaquette is $\phi/3$. Therefore, the Peierls substitution happens to be just a gauge transformation only when $\phi = 3n\phi_0$, with $n$ integer.

V. CONCLUSIONS

We have studied the electronic behavior of a graphene bilayer using the minimal tight-binding model that describes the system. Particular focus has been given to
the presence of an external electric field perpendicular to the bilayer system—biased bilayer—which gives rise to a finite gap in the spectrum, whose size is controlled solely by the applied voltage. The effect of the perpendicular electric field has been included through a parallel plate capacitor model, with screening correction at the Hartree level. The model has been applied to real biased bilayer devices, either made out of SiC or exfoliated graphene. The good agreement with experimental results—namely, for the electrostatic energy difference between layers obtained through ARPES for the Shubnikov-de Haas cyclotron mass and for the presence of a new Hall plateau at zero Hall conductivity—clearly indicates that the model is capturing the key ingredients, and that a finite gap is effectively being controlled externally. The biased bilayer thus realizes the first tunable gap semiconductor—a proof of principle regarding real applications of graphene bilayer. Analysis of recent experimental results regarding the electrical noise and cyclotron resonance further suggests that the model can be seen as a good starting point to understand the electronic properties of graphene bilayer. We have compared the full tight-binding description with its 4-band and 2-band continuum approximations, and found that the 4-band model is always a suitable approximation for the conditions realized in experiments. Also, we have studied the effect of electron-hole asymmetry terms, as the second-nearest-neighbor hopping energies \( t' \) (in-plane) and \( \gamma_4 \) (inter-layer), and the on-site energy \( \Delta \), and found that they have only a small effect on the electronic properties addressed here.

\[ \Delta = \Delta_n + \Delta_n' \]  
[\( \Delta_n' \) is the fluctuation of the charge density.]

**Acknowledgments**


**APPENDIX A: ASYMMETRY BETWEEN LAYERS**

In order to write Eq. (A3) as an energy integral, we start by introducing the SLG density of states per spin per unit cell defined for the conduction band as

\[ \rho(\epsilon) = \frac{1}{N_c} \sum_k \delta(\epsilon - t|s_k|), \quad (A1) \]

with \( s_k \) given by Eq. (A5). The momentum sum in Eq. (A1) is over the BZ defined in Fig. 2 and can be written as an integral by letting \( N_c \rightarrow \infty \). The integral can be performed, leading to

\[ \rho(\epsilon) = \frac{2\epsilon}{t^2 \pi^2} \left\{ \begin{array}{ll} \frac{1}{\sqrt{F(\epsilon/t)}} K \left( \frac{4\epsilon/t}{F(\epsilon/t)} \right), & 0 < \epsilon < t \\ \frac{1}{\sqrt{F(\epsilon/t)}} K \left( \frac{4\epsilon/t}{F(\epsilon/t)} \right), & t < \epsilon < 3t \end{array} \right., \quad (A2) \]

where \( F(x) \) is given by

\[ F(x) = (1 + x)^2 - \frac{(x^2 - 1)^2}{4}, \quad (A3) \]

and \( K(m) \) is the complete elliptic integral of the first kind,

\[ K(m) = \int_0^1 \frac{1}{\sqrt{(1 - x^2)(1 - mx^2)}} \, dx \quad (A4) \]

With the definition of \( \rho(\epsilon) \) in Eq. (A1), it is readily shown that the charge imbalance between layers in Eq. (A5) can be written as

\[ \Delta n = \Delta n_{1/2} + \Delta n', \quad (A5) \]

where the charge imbalance at half-filling \( \Delta n_{1/2} \) is given by

\[ \Delta n_{1/2} = \frac{2}{A_0} \sum_{l=0}^3 \int_0^{3L} d\epsilon \rho(\epsilon) I^{-l}(\epsilon), \quad (A6) \]

and the fluctuation \( \Delta n \) with respect to the half-filled case is given by
\[
\Delta \bar{n} = \frac{2}{A_0} \left\{ \sum_{l=\pm} \int_{E_{F}}^{E_{F}^{n}} d\rho(\epsilon) \mathcal{I}^+(\epsilon), \quad n > 0 \right\} - \left\{ \sum_{l=\pm} \int_{E_{F}}^{E_{F}^{n}} d\rho(\epsilon) \mathcal{I}^{-}(\epsilon), \quad n < 0 \right\}, \quad (A7)
\]

where \( n \) is the carrier density with respect to half-filling. The integral kernel in Eqs. (A6) and (A7) reads

\[
\mathcal{I}^\pm(\epsilon) = \frac{[\epsilon^2 + K^\pm_+ \pm (\epsilon^2 - K^\pm_+)]^2 - (\epsilon^2 + K^\pm_+)^2 K^\pm_2(\epsilon)}{[\epsilon^2 + K^\pm_+][\epsilon^2 - K^\pm_+]^2 + [\epsilon^2 + K^\pm_+]^2 K^\pm_2(\epsilon)}, \quad (A8)
\]

where \( K^\pm_+ = [V/2 \pm E^\pm(E)]^2 \), with \( E^\pm(E) \) given by Eq. (19) with the substitution \( \epsilon_k \rightarrow \epsilon \). The limits of integration in Eq. (A7) depend on the band label \( l \) and Fermi energy \( E_F \) as follows: for \( l = - \) we have \( \epsilon_1 = \epsilon^- \) and \( \epsilon_2 = \epsilon^+ \) for \( E_F^2 < V^2/4 \), while for \( E_F^2 > V^2/4 \) we have \( \epsilon_1 = 0 \) and \( \epsilon_2 = \epsilon^+ \); with \( l = + \) we only have

\[
\rho_2^-(E) = \frac{4}{t^2 \pi^2} \begin{cases} 
\frac{\psi^{-}(E)}{\sqrt{F(\epsilon^{-}(E)/t)}} K \left( \frac{4\epsilon^{-}(E)/t}{F(\epsilon^{-}(E)/t)} \right), & \left\{ \begin{array}{l}
\Delta_g/2 < |E| < V/2 \land \alpha \leq t^2 \\
E^+(t) < |E| < V/2 \land \alpha > t^2
\end{array} \right. \\
\frac{\psi^{+}(E)}{\sqrt{F(\epsilon^{+}(E)/t)}} K \left( \frac{4\epsilon^{+}(E)/t}{F(\epsilon^{+}(E)/t)} \right), & \Delta_g/2 < |E| < E^+ - (t) \land \alpha < t^2
\end{cases}
\]

and

\[
\rho_2^+(E) = \frac{4}{t^2 \pi^2} \begin{cases} 
\frac{\psi^{-}(E)}{\sqrt{F(\epsilon^{-}(E)/t)}} K \left( \frac{4\epsilon^{-}(E)/t}{F(\epsilon^{-}(E)/t)} \right), & \sqrt{t^2_1 + V^2/4} < |E| < E^+(t), \\
\frac{\psi^{+}(E)}{\sqrt{F(\epsilon^{+}(E)/t)}} K \left( \frac{F(\epsilon^{+}(E)/t)}{4\epsilon^{+}(E)/t} \right), & E^+(t) < |E| < E^+ + (3t) \land t^2 \leq \alpha < 9t^2
\end{cases}
\]

with \( \psi^{\pm}(E) \) and \( \chi^{\pm}(E) \) respectively given by

\[
\psi^{\pm}(E) = \sqrt{t^4_1/4 + (t^2_1 + V^2)^2} \chi^{\pm}(E)^2 \sqrt{\chi^{\pm}(E)}^2 + t^2_1/2 + V^2/4 \pm \sqrt{t^4_1/4 + (t^2_1 + V^2)^2} \chi^{\pm}(E) \chi^{\pm}(E)^2 \pm (t^2_1 + V^2)^2/2}
\]

and

\[
\chi^{\pm}(E) = \sqrt{E^2 + V^2/4 \pm \sqrt{E^2(V^2 + t^2_1) - t^2_1 V^2/4}}, \quad (B5)
\]

where the functions \( F(x) \) and \( K(x) \) are given by Eqs. (A3) and (A3), respectively, and \( E^{\pm\pm}(x) \) is given by Eq. (19) with the substitution \( \epsilon_k \rightarrow x \) and \( \alpha = \]
(V^4/4 + t_\perp^4 V^2/2)/(V^2 + t_\perp^2).

APPENDIX C: CYCLOTRON MASS

Based on the full tight-binding band structure $E_\mathbf{k}^{\pm\pm}$
given in Eq. (19), it is possible to derive general expressions
for the cyclotron mass in Eq. (60). The key observation is that
the area of a closed orbit at the Fermi level $A(E_F)$ may be
written as $A(E_F) \propto \sum \Delta_k$, where the prime means
summation over all k’s inside the orbit, and $\Delta_k = (2\pi)^2/(N_x A_y)$
the area per k-point in the first BZ. The cyclotron mass then be written as

$$m_c(E_F) = \frac{\hbar^2}{A_c t^2 \pi} \left| \frac{-\psi^-(E_F)}{F[\psi^-(E_F)]} \right|^2 K \left( \frac{4\Delta^2}{F[\psi^-(E_F)]} \right) \Delta_g/2 < |E_F| < V/2$$

$$\psi^+(E_F) \frac{\gamma^+(E_F)}{F[\psi^+(E_F)]} K \left( \frac{4\gamma^2}{F[\psi^+(E_F)]} \right) \Delta_g/2 < |E_F| \lesssim t$$

$$\psi^-(E_F) \frac{\gamma^-(E_F)}{F[\psi^-(E_F)]} K \left( \frac{4\gamma^2}{F[\psi^-(E_F)]} \right) \sqrt{t_\perp^2 + V^2}/4 < |E_F| \lesssim t$$

where $\psi^{\pm\mu}(E)$ and $\gamma^{\pm}(E)$ are given by Eqs. (13) and (15), $F(x)$ is given by Eq. (13), and $K(m)$ is
the complete elliptic integral of the first kind defined in
Eq. (13).

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