Van der Waals heterostructures are promising new materials which have been drawing increasingly attention [1–4]. In this work, we focus on the theoretical description of one of the simplest stackings, the twisted bilayer graphene, which can be seen as one of the fundamental pieces for more complex assemblies. Starting from a single-particle theory, based on a low-energy continuum model [5], we address the optical properties, namely the optical conductivity (within the linear response theory) and the spectrum of graphene surface plasmon-polaritons (using a semi-classical treatment). As our own contribution, we highlight the introduction of a new and improved method for computing the Drude conductivity and the obtention of original results for the plasmonic response (transverse magnetic modes) of this system.

Keywords: twisted bilayer graphene, low-energy continuum model, optical conductivity, surface plasmon-polaritons.

I. INTRODUCTION

Two-dimensional (2D) crystals have attracted widespread attention of the scientific community, especially since their first experimental isolation in 2004 [5]. Amongst them, graphene—a 2D honeycomb lattice of carbon atoms—has stood out, leading to the development of a research area of its own [7–9]. In parallel with the efforts being made on graphene and other 2D materials, a new research field dealing with van der Waals (vdW) heterostructures—artificial three-dimensional (3D) structures made by stacking 2D crystals together (fig. 1)—has recently emerged [1–3]. Within this approach, the aim is to design heterostructures that exhibit tailored properties for technological applications. In this work, the focus is on one of the simplest stackings, the twisted bilayer graphene (tBLG)—a graphene sheet on top of another, with a twist angle $\theta$—, which can be seen as one of the fundamental pieces for more complex assemblies.

The complex geometry of the tBLG affects significantly its electronic properties, making even the single-particle models quite involved [10]. This geometry is characterized by the twist angle $\theta$, which manifests itself in the appearance of a moiré pattern revealing the periodicity (or quasiperiodicity) of the crystal structure [11]. While the moiré exists for any $\theta$, the superstructure, that is, strickly periodic repetition of some large multiatomic supercell, occurs only for the so-called commensurate angles [12]. For commensurate structures, numerical studies based on density functional theory (DFT) have been performed [13–15]. However, since the unit cell of the tBLG superlattice contains a large number of sites, especially at small $\theta$, these $ab$ initio calculations incur a significant computational cost and are therefore rather unpractical. To avoid this difficulty, semi-analytical theories have been developed in order to describe the low-energy electronic properties of the tBLG [5, 12, 16–18].

In general, the study of light-matter interactions is a topic of interest in science, with a wide variety of applications, for example in the field of photonics. For graphene, and in particular for the tBLG, the response to an applied electromagnetic field is characterized by the optical conductivity, which has been computed using analytical [19, 20] and numerical [21] models. Over the last few years, graphene plasmonics has also emerged as a new topic [22], especially after the experimental realization achieved by the end of 2011, when Ju et al. [23] showed the possibility of exciting graphene surface plasmon-polaritons (GSPPs) in the THz spectral range by shining electromagnetic radiation onto a periodic grid of graphene micro-ribbons. The major advantage of using graphene as the surface for the propagation of these plasmon-polaritons relates essentially with the strong confinement [24, 25] and the easy tunability [26–28] of the collective excitations. Within a semi-classical treatment [29], the dispersion relation of GSPPs depends
explicitly on the optical conductivity, wherefore the study of
their spectrum — which, for the tBLG system, is an ab-
sent topic in literature — follows as a direct application.

In this work, we start by reproducing, in section III the
continuum model developed by Bistritzer and MacDonald [5],
which is valid for $\theta \lesssim 10^7$ and independent of the
structure being commensurate or incommensurate. In
section IV we address the optical conductivity (within
the linear response theory), comparing our results and
methods with the current literature. Section V contains
original results for the transverse magnetic (TM) modes
of GSPPs, which were obtained making use of the pre-
vious calculations. Finally, in section VI we present our
main conclusions and proposals for future work.

II. LOW-ENERGY CONTINUUM MODEL

A. Folded description for single layer graphene

Before moving to the derivation of the continuum
model, we first look into the folded description of the
single layer graphene (SLG), since it will provide us a
better understanding of that approach.

We start with SLG basics. The geometry (fig. 2) is
defined by the following hexagonal lattice which describes
the positions for the unit cells of this system:

$$R_{n_1,n_2} = n_1 a_1 + n_2 a_2, \quad n_1,n_2 \in \mathbb{Z},$$

in which the primitive vectors $a_1$ and $a_2$ are given by

$$a_1 = (1/2, \sqrt{3}/2) \sqrt{3} d, \quad a_2 = (-1/2, \sqrt{3}/2) \sqrt{3} d.$$

Given this lattice, we define the corresponding $k$-space
(fig. 3) by writing the reciprocal lattice as

$$G_{m_1,m_2} = m_1 b_1 + m_2 b_2, \quad m_1,m_2 \in \mathbb{Z},$$

where the reciprocal primitive vectors $b_1$ and $b_2$ are given by

$$b_1 = \left(\sqrt{3}/2,1/2\right) \frac{4\pi}{3d}, \quad b_2 = \left(-\sqrt{3}/2,1/2\right) \frac{4\pi}{3d}.$$

Within the tight-binding model, the SLG Hamiltonian
for hopping $-t$ ($t = 2.97eV$ [3]) between first nearest
neighbors (NN) is given by [8]

$$H(k) = \begin{bmatrix}
0 & -tf(k) \\
-tf^*(k) & 0
\end{bmatrix}, \quad (1)$$

where

$$f(k) = e^{ik\delta} (1 + e^{-ik}a_1 + e^{-ik}a_2),$$

with $\delta = (0, d)$ being the vector that links the 2 atoms in
the same unit cell.

![SLG geometry](image)

**FIG. 2:** SLG geometry. The honeycomb structure can be seen as two interpenetrating hexagonal lattices, A (blue) and
B (red). Its experimental structural parameter, the carbon-carbon distance, is $d = 1.42Å$ [8]. The dashed green line
marks a unit cell of this system, which contains 2 atoms. The
coordinate system is centered at a carbon of sublattice A.

The folded description lays in the observation that we
can opt for larger direct lattices, as long as they still
capture the system’s periodicity. In the simpler case in
which we choose unit cells $3p$ ($p \in \mathbb{N}$) times larger than
the original one, which corresponds to folding the BZ to
$1/3p$ of its previous size, we obtain

$$a_1^{(p)} = \begin{cases}
(1/2, \sqrt{3}/2) \sqrt{3}^{p+1} d & \text{if } p \text{ is even} \\
(\sqrt{3}/2,1/2) \sqrt{3}^{p+1} d & \text{if } p \text{ is odd}
\end{cases},$$

$$a_2^{(p)} = \begin{cases}
(-1/2, \sqrt{3}/2) \sqrt{3}^{p+1} d & \text{if } p \text{ is even} \\
(-\sqrt{3}/2,1/2) \sqrt{3}^{p+1} d & \text{if } p \text{ is odd}
\end{cases},$$

$$b_1^{(p)} = \begin{cases}
(\sqrt{3}/2,1/2) \frac{4\pi}{3^{p+1}d} & \text{if } p \text{ is even} \\
(1/2,\sqrt{3}/2) \frac{4\pi}{3^{p+1}d} & \text{if } p \text{ is odd}
\end{cases},$$

$$b_2^{(p)} = \begin{cases}
(-\sqrt{3}/2,1/2) \frac{4\pi}{3^{p+1}d} & \text{if } p \text{ is even} \\
(-1/2,\sqrt{3}/2) \frac{4\pi}{3^{p+1}d} & \text{if } p \text{ is odd}
\end{cases}.$$
We start by defining the matrix element,

\[ T_{\mathbf{k}, \mathbf{k}'}^{\alpha, \beta} = \langle \psi_{\mathbf{k}, \alpha}^{(1)} | H_{\perp} | \psi_{\mathbf{k}', \beta}^{(2)} \rangle, \]

which describes a process where an electron with momentum \( \mathbf{k}' \) in layer 2, sublattice \( \beta \), hops to a momentum state \( \mathbf{k} \) in layer 1, sublattice \( \alpha \). In the tight-binding ap-
FIG. 5: tBLG geometry for \( \theta = 5^\circ \) and \( \tau = 0 \) (top view). Vectors \( \mathbf{a}_1^m \) and \( \mathbf{a}_2^m \) mark the basis for the (readily visible) large-scale hexagonal moiré pattern. The typical interlayer distance is \( d_\perp = 3.35 \text{Å} \) [10].

proximation, we have

\[
\begin{align*}
|\psi_{\alpha}^{(1)}(k)\rangle &= \frac{1}{\sqrt{N}} \sum_{n_1,n_2} e^{i\mathbf{k} \cdot \mathbf{R}_{n_1,n_2}^{(1)} + \delta_{\alpha}(\mathbf{R}_{n_1,n_2}^{(1)},\alpha)}, \\
|\psi_{\beta}^{(2)}(k)\rangle &= \frac{1}{\sqrt{N}} \sum_{n_1,n_2} e^{i\mathbf{k} \cdot \mathbf{R}_{n_1,n_2}^{(2)} + \delta_{\beta}(\mathbf{R}_{n_1,n_2}^{(2)},\beta)},
\end{align*}
\]

where \( N \) stands for the total number of unit cells and

\[
\delta_{\alpha}^{(1)} = \delta_\alpha, \quad \delta_{\beta}^{(2)} = \delta_\beta,
\]

with \( \delta_A = 0 \) and \( \delta_B = \delta \). Invoking the two-center approximation,

\[
\begin{align*}
\langle R_{n_1,n_2}^{(1)} + \delta_{\alpha}^{(1)},\alpha | H_{\perp} | R_{n_1,n_2}^{(2)} + \delta_{\beta}^{(2)},\beta \rangle \\
= t_\perp (R_{n_1,n_2}^{(1)} + \delta_{\alpha}^{(1)} - R_{n_1,n_2}^{(2)} - \delta_{\beta}^{(2)}),
\end{align*}
\]

we can calculate the following matrix element (which is, for now, completely general):

\[
T_{\alpha\beta}^{m,n,m+n} = \sum \frac{t_\perp (K + q_1 + G_{k,l})}{A_{g.u.c.}} \times e^{i(G_{k,l} \cdot \mathbf{a}_m - G_{m,n} \cdot (\delta_{\beta} - \delta))} \delta_{K+q_1+G_{k,l}+q_{\perp}+q_{\parallel}+G_{m,n} = 0},
\]

where \( A_{g.u.c.} = \frac{3\sqrt{3}}{2} \) is the area of a SLG unit cell and \( t_\perp (\mathbf{k}) \) is the Fourier transform (FT) of the interlayer tunneling amplitude, \( t_\perp (\mathbf{k}) \). We stress that we have already set \( \tau = 0 \) since the spectrum is known to be \( \tau \)-independent for \( \theta \neq 0 \) [2].

Taking a look at this expression, we notice that the moiré pattern reveals itself in the

Kronecker delta, \( \delta_{K+q_1+G_{k,l}+q_{\perp}+q_{\parallel}+G_{m,n} = 0} \), which dictates that the momentum difference in the interlayer hopping must be a vector resulting from the union of all vectors \( \mathbf{G} \) and \( \mathbf{G}^\theta \).

The continuum low-energy model is obtained by considering wave vectors in both layers relative to their respective Dirac points with small deviations compared to the BZ dimensions: \( |q_1|, |q_2| \ll |K| \). Notice that, by doing so, a \( K \) expansion is implicit at this point. The model’s usefulness rests on the numerical results obtained for \( t_\perp (\mathbf{k}) \) (fig. 3), which indicate that it should fall to zero very rapidly with \( |\mathbf{k}| \) on the reciprocal lattice scale. Keeping the dominant terms from the FT, we get

\[
T_{K+q_1, \alpha}^{m,n} q_\parallel^m + q_\perp^m = \frac{1}{A_{g.u.c.}} T_{q_{\parallel}}, \delta_{q_{\parallel} - q_{\parallel} = 0} + T_{q_{\perp}}, \delta_{q_{\parallel} - q_{\parallel} = 0} + T_{q_{\perp}}, \delta_{q_{\parallel} - q_{\parallel} = 0},
\]

with

\[
T_{q_{\parallel}} = \frac{t_\perp (K)}{A_{g.u.c.}} T_1, \quad T_{q_{\perp}} = \frac{t_\perp (K)}{A_{g.u.c.}} T_2, \quad T_{q_{\perp}} = \frac{t_\perp (K)}{A_{g.u.c.}} T_3,
\]

\[
T_1 = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}, \quad T_2 = \begin{bmatrix} e^{i\phi} & 1 \\ e^{-i\phi} & 1 \end{bmatrix}, \quad T_3 = \begin{bmatrix} e^{i\phi} & 1 \\ e^{-i\phi} & 1 \end{bmatrix},
\]

\( \phi = \frac{2\pi}{3} \), and

\[
q_{\parallel} = K - K^\theta, \quad q_{\perp} = q_{\parallel} + b_{\perp}^m, \quad q_{\parallel} = q_{\parallel} - b_{\parallel}^m.
\]

The parameter \( t_\perp (\mathbf{k}) \) is fixed by taking the limit \( \theta \to 0 \) and comparing the resulting interlayer hopping term, \( 3 \frac{t_\perp (K)}{A_{g.u.c.}} \delta_{\beta,m} b_{\parallel}^m \mathbf{q}_{\parallel} \), with the known results for the AB stacked bilayer graphene [10]: this yields the relation \( 3 \frac{t_\perp (K)}{A_{g.u.c.}} = t_\perp^\text{AB} \), where \( t_\perp^\text{AB} = 330 \text{meV} \) is the hopping term between an \( A \) site from layer 1 and the NN \( B \) site from layer 2 in the AB stacked configuration.

The interpretation of this model is more elegant when we move to the reference frame where layer 1 is rotated by \( -\theta/2 \) and layer 2 by \( \theta/2 \) (it suffices to rotate our previous coordinate system by \( \theta/2 \)). The geometrical picture for this interlayer hopping is explained in fig. 7.
reads

\[ (H_1 + H_2 + H_3) |\psi_k\rangle = E |\psi_k\rangle, \]

where \( H_i \) is the Hamiltonian for layer \( i \) (\( i = 1, 2 \)), \( E \) is the energy and

\[ |\psi_k\rangle = \sum_{\alpha, \beta} c^{(i)}_{\alpha}(k) |\psi^{(i)}_{k, \alpha}\rangle \]

is the total wave function, with \( c^{(i)}_{\alpha}(k) \) standing for a complex constant of unit modulus. The interlayer hopping matrix elements are modelled by eq. (3) whereas, for the intralayer ones, we use each layer’s (rotated) Dirac Hamiltonian, eq. (2). We thus realize that we can never get a closed system of equations by applying bras, \( \langle \psi^{(i)}_{k, \alpha} | \equiv \langle k, i, \alpha | \) : if we start, for example, with the bra \( \langle K + q, 1 | \) (dropping the index of sublattice), we will have, aside from the diagonal term, reciprocal space hopping terms (matrix elements) with states \( |K^\theta + q + q_0, 2\rangle\), \( |K^\theta + q + q_{tr}, 2\rangle\) and \( |K^\theta + q + q_{tl}, 2\rangle\) (we will call them the first NN in reciprocal space, in lack of better terminology); in turn, each one of these will have hopping terms with the former one and with two new states (second NN), and so on (recall the picture shown in fig. 7b). To clarify this matrix construction, we present the simpler example in table I in which we start with the bra \( \langle K + q, 1 | \) and consider just first NN.

In this matrix construction, we point out the similarities with what was shown for the folded SLG (section II A). In fact, if we eliminate the interlayer hopping terms (i.e., the non-diagonal matrix elements), we are basically using a folded description that explicitly captures the moiré periodicity to some extent (depending on the truncation). In real space, the interpretation is that we are using an enlarged unit cell with the moiré periodicity. Obviously, this is not as elegant as the case of the 1/3\( \pi \) SLG folding which could always be written as a finite dimension matrix that captured the periodicity for all momenta. The major difference is that we are now using a Dirac approximation. For this reason, we should also be aware that we will obtain high-energy bands lacking physical meaning; however, this should not constitute a major problem since we are not interested in them anyway. When we add the hopping terms, we see that, the more we add, the less important we expect them to be. Nevertheless, we cannot always stick to first NN hopping terms only, because, depending on the angle, the low-energy bands may still depend on high-order NN hopping processes. This is the balance we have to test.
numerically in order to truncate our (in principle infinite) matrix. With all the approximations, this model is expected to be very accurate up to energies of $\sim 1$ eV, which can still capture the first low-energy bands for $\theta \lesssim 10^\circ$.

F. Electronic spectrum

Before moving to the band spectrum determination, it is crucial to recall that our Hamiltonian was obtained within a low-energy expansion around $K$. Yet, nothing prevents us to choose the other nonequivalent Dirac point, $K'$, for which the deductions are completely analogous. Therefore, in order to describe the complete electronic properties of this material, we should always consider both contributions, usually called $K$ and $K'$ bands. The way to represent both $K$ and $K'$ bands in the same BZ is sketched in fig. 8. We notice that, in a $K$ expansion, the wave vector $\mathbf{q}$ is measured from $K^{(1)}$ ($\mathbf{k} = K^{(1)} + \mathbf{q}$) while, in a $K'$ expansion, we measure it from $K'^{(1)}$. Therefore, in order to match both moiré unit cells in reciprocal space (purple and green), we identify the points $K^{(1)}$ and $K'^{(2)}$ as the same point in the moiré BZ, such that the path $K_m \rightarrow K'_m \rightarrow M_m \rightarrow K_m$ becomes equivalent. By doing so, we are making a correspondence $\mathbb{H}^K_{tBLG}(\mathbf{q}) \leftrightarrow \mathbb{H}^{K'}_{tBLG}(\mathbf{q} + \mathbf{q}_b)$ in the Hamiltonians obtained within $K$ and $K'$ expansions.

Results for electronic spectrum, density of states (DOS) and carrier density are plotted in figs. 9, 10. Looking at the spectrum, we observe an apparent symmetry for positive and negative bands. We also see a renormalization of the Fermi velocity, which is explored in more detail in refs. [5, 16]. Addressing fig. 10 we conclude that, by varying the twist angle, van Hove singularities can be brought to accessible energies, which is one of the main features of the tBLG [32]. For the carrier density, we highlight that we start to lose the “signature behavior” of the decoupled bilayer graphene (BLG) when we reach small angles.
### III. OPTICAL CONDUCTIVITY

#### A. Linear response theory

Within the linear response theory, the (dynamical) total conductivity tensor, \( \sigma_{\alpha \beta}(\omega) \) \((\alpha, \beta = x, y)\), can be split into two terms,

\[
\sigma_{\alpha \beta}(\omega) = \sigma^D_{\alpha \beta}(\omega) + \sigma^{reg}_{\alpha \beta}(\omega),
\]

where \( \sigma^D(\omega) \) is the Drude conductivity—an intraband contribution (in which momentum is not conserved) that reflects the response of the electrons to a static applied electric field—and \( \sigma^{reg}(\omega) \) is the regular conductivity—an interband contribution which corresponds to electronic band transitions (within the same \( k \)) with energy \( h\omega \), induced by an applied harmonic electric field, \( E \sim e^{-i\omega t} \) (\( t \) is the time, \( \omega \) is the angular frequency).

For the Drude term, our derivation yielded

\[
\sigma^D_{\alpha \beta}(\omega) = \frac{i}{\pi} \frac{D_{\alpha \beta}}{h\omega + i\Gamma},
\]

where \( \Gamma \) is an empirical broadening parameter (usually interpreted as a scattering rate) that accounts for disorder effects (impurities, electron-electron interactions, substrate, etc.) and \( D_{\alpha \beta} \) is the Drude weight tensor, given by

\[
D_{\alpha \beta} = \frac{8\pi\sigma_0}{N_{A_{u.c.}}} \sum_{k \in BZ, \lambda} \left[ \langle \lambda_1, k | j_{\alpha 1 \beta 2} | \lambda_1, k \rangle n_F(\epsilon_{\lambda_1}(k)) + \sum_{\lambda_2 \neq \lambda_1} \langle \lambda_1, k | j_{\alpha 1 \beta 2} | \lambda_2, k \rangle \langle \lambda_2, k | j_{\beta 2 \alpha 1} | \lambda_1, k \rangle \right. \\
\times \left. \frac{n_F(\epsilon_{\lambda_2}(k)) - n_F(\epsilon_{\lambda_1}(k))}{\epsilon_{\lambda_1}(k) - \epsilon_{\lambda_2}(k)} \right].
\]

In the last expression, \( \sigma_0 = e^2/(4\hbar) \) is the graphene universal conductance \( e \) being the elementary charge, \( A_{u.c.} \) is the area of a unit cell and \( n_F \) is the Fermi-Dirac function for some Fermi level \( \mu \) and temperature \( T \). Moreover, we have \( j_{\alpha 1} \equiv \frac{\partial H_0(k)}{\partial k_{\alpha 1}} \) and \( j_{\alpha 2}^2 \equiv \frac{\partial^2 H_0(k)}{\partial k_{\alpha 1} \partial k_{\alpha 2}} \), where \( H_0 \) is a (general) spin-independent tight-binding Hamiltonian matrix for a periodic system, with eigenvalues \( \epsilon_{\lambda}(k) \) and eigenvectors \( |\lambda, k\rangle \) for momentum \( k \) and band \( \lambda \). We also stress that eq. (4) already takes into account the spin degeneracy. As for the valley degeneracy (for the tBLG case), we clarify that it is implicit in the sum over \( k \in BZ \), which should be done into two sums over \( q \) in moiré BZs centered around \( K \) and \( K' \).

For the regular contribution, we obtained

\[
\sigma^{reg}_{\alpha \beta}(\omega) = \frac{8\pi\sigma_0}{N_{A_{u.c.}}} \sum_{k \in BZ, \lambda} \langle \lambda_1, k | j_{\alpha 1 \beta 2} | \lambda_1, k \rangle \langle \lambda_2, k | j_{\beta 2 \alpha 1} | \lambda_1, k \rangle \times \\
\times \frac{n_F(\epsilon_{\lambda_1}(k)) - n_F(\epsilon_{\lambda_2}(k))}{[\epsilon_{\lambda_1}(k) - \epsilon_{\lambda_2}(k)] [\epsilon_{\lambda_1}(k) - \epsilon_{\lambda_2}(k)] + h\omega + i\Gamma}.
\]

#### B. Alternative methods

Eqs. (4) and (5) must work when we have the complete Hamiltonian defined in the full BZ (this was actually verified by computing the results for the SLG). However, as we shall discuss, for effective Hamiltonians (which is the case we are interested in), they might not be the most appropriate. In this section, we thus provide alternative methods to compute these quantities.

When determining the Drude weight, we expect that all the dependency comes from the electrons near the Fermi level, which are the ones that can flow in response to the static applied electric field. Yet, this is not explicit in eq. (4), which indicates that there should be an underlying annulment of the other terms. In fact, with some manipulation of this equation, we can arrive to

\[
D_{\alpha \beta} = \frac{8\pi\sigma_0}{N_{A_{u.c.}}} \sum_{k \in BZ, \lambda} \frac{\partial \epsilon_\lambda(k)}{\partial k_{\alpha 1}} \frac{\partial \epsilon_\lambda(k)}{\partial k_{\alpha 2}} \frac{\partial n_F(\epsilon)}{\partial \epsilon} (\epsilon_{\lambda}(k) - \epsilon_{\lambda_1}(k)),
\]

which is clearly a better method, since the derivative of the Fermi-Dirac is very sharp around \( \epsilon \sim \mu \).

Regarding the regular conductivity (eq. (5)), we observe that the real part is strongly constrained to eigen-
states within $\hbar \omega$ of the Fermi level. Hence, this computation should not be problematic and we will keep this method. For the imaginary part, we see that, even for small $\omega$, we do not have an argument to avoid a summation over all the bands. Therefore, following the work done in ref. [20], we may think of using the Kramers-Kronig (KK) relations [33] to compute the imaginary part using the results for the real part,

$$\text{Im} \{\sigma^{\text{reg}}(\omega)\} = -\frac{2\omega}{\pi} P \int_0^{+\infty} ds \frac{\text{Re} \{\sigma^{\text{reg}}(s)\}}{s^2 - \omega^2}. \quad (7)$$

Looking at this expression, there is yet no clear advantage in using this strategy, since the integral extends to infinity. Moreover, this integral is ill defined, since at high frequencies our continuum model for the tBLG is expected to yield a constant $\text{Re} \{\sigma^{\text{reg}}(\omega)\} = 2\sigma_0$. We can thus perform a regularization of eq. (7) by invoking the following property (which we verified numerically):

$$P \int_0^{+\infty} ds \frac{1}{s^2 - \omega^2} = 0.$$

The final regularized definition then reads

$$\text{Im} \{\sigma^{\text{reg}}(\omega)\} = -\frac{2\omega}{\pi} P \int_0^{+\infty} ds \frac{\text{Re} \{\sigma^{\text{reg}}(s)\} - 2\sigma_0}{s^2 - \omega^2}. \quad (8)$$

which we can now evaluate by introducing a finite cutoff $\Lambda$ for which $\text{Re} \{\sigma^{\text{reg}}(\Lambda)\} \simeq 2\sigma_0$. We also remark that, although our model yields a constant for high frequencies, it is not problematic in the range of frequencies in which we are interested in.

C. Results

Some of the results obtained for the Drude weight in tBLG systems are summarized in fig. 11. As anticipated, only the 2nd method (eq. (6)) worked well. We observe symmetric outcomes for electron or hole doping; this reflects the apparent symmetry in positive and negative bands discussed in section [17]. By looking at fig. 11a along with fig. 10a we conclude that the Drude weight curve changes drastically (compared with SLG or decoupled BLG) when we cross the van Hove singularities; this tendency coincides with what was found in ref. [20]. The effect of increasing the temperature is the smoothening of this behavior (fig. 11b).

In figs. 12, 13, we show representative results that allow us to analyze the regular conductivity in tBLG systems. All conductivity results obtained were isotropic. Looking at fig. 12a, we first notice the expected dependency on both the Fermi level and temperature; transitions with $\hbar \omega \lesssim 2\mu$ are Pauli blocked and the decreasing of $T$ accentuates this behavior. In addition, we observe a low-energy peak (marked with a green arrow), which we interpret as the dominant transitions shown in fig. 12b. Notice that there are other transitions (red and orange arrows) which we would expect to be dominant, since they connect different van Hove singularities; however, these ones are optically inactive, in agreement with what was found in refs. [19, 21]. This optical selection rule occurs due to a symmetry in the effective Hamiltonian which makes the matrix elements from eq. (5) null for bands with symmetric energies and in the $M_m$ points only [21]. From fig. 13a, we highlight the fact that the results obtained for the decoupled tBLG —tBLG with $t_{\perp} = 0$— match perfectly the results for $2\times$SLG (results for SLG, multiplied by 2). Although this was trivially expected, it was only achieved when we used the 2nd method for computing the imaginary part of the regular conductivity (eq. (8)); therefore, this served as a benchmark test for the validity of this method. Moreover, we remark that we now have a region with a big deep on $\text{Im} \{\sigma^{\text{reg}}(\omega)\}$ occurring at lower frequencies, which will be an important feature in section [17]. Regarding fig. 13b, we emphasize that, for small angles, we start to lose the “signature” behavior of the curves because of the presence of multiple low-energy van Hove singularities.
IV. SPECTRUM OF GRAPHENE SURFACE PLASMON-POLARITONS — TRANSVERSE MAGNETIC MODES

We consider a system consisting of a single graphene sheet cladded between two semi-infinite dielectric media, characterized by the real dielectric constants (relative permittivities) $\varepsilon_1^r$ and $\varepsilon_2^r$, as depicted in fig. 14. We stress that, although the tBLG is not truly a 2D surface, its thickness is still negligible and we can view it as a monolayer for these purposes [7].

Assuming, for each medium $j = 1, 2$, a solution of Maxwell’s equations in the form of a TM wave, confined to the neighborhood of the graphene sheet (with damping parameter $\kappa_j$), propagating along the $\hat{x}$-direction, and of the typical harmonic form, we obtain the following dispersion relation [29]:

$$\frac{\varepsilon_1^r}{\kappa_1(q, \omega)} + \frac{\varepsilon_2^r}{\kappa_2(q, \omega)} + \frac{i}{\omega \varepsilon_0} \sigma(\omega) = 0,$$

(9)

which results from imposing the continuity of the tangential component of the electric field and the discontinuity of the tangential component of the magnetic field across the interface. In this equation, $\varepsilon_0$ is the vacuum permittivity, $\sigma(\omega) \equiv \sigma_{xx} = \sigma_{yy}$ (valid for unstrained graphene) is the total conductivity, $q \equiv q_1 = q_2$ is the momentum of the electromagnetic wave propagating in each medium (which must be conserved due to translational invariance) and $\kappa_j(q, \omega)$ is given by:

$$\kappa_j(q, \omega) = \sqrt{q^2 - \frac{\omega^2 \varepsilon_j^r}{c^2}},$$

where $c$ is the speed of light. Eq. (9) describes the dispersion relation, $\omega(q)$, of graphene TM surface plasmon-polaritons. Notice that this is an implicit equation, so it needs to be solved numerically. Nonetheless, we easily see that it is only solvable when $\text{Im}\{\sigma(\omega)\} > 0$. 

FIG. 12: tBLG with $\theta = 9^\circ$: (a) real part of the regular conductivity; (b) spectrum. In (a), the dotted blue line corresponds to $T = 100$K, the dashed blue line to $T = 200$K and the solid lines to $T = 300$K; the black dashed line is for decoupled tBLG (or $2 \times$SLG) at $T = 300$K and $\mu = 0$. The broadening parameter $\Gamma$ was set as $\Gamma = 16$meV in agreement with ref. [23].

FIG. 13: Regular conductivity results for tBLG. In (a) and (b), the dashed lines are for decoupled BLG or $2 \times$SLG.

FIG. 14: Illustration of a single graphene sheet sandwiched between two semi-infinite insulators with relative permittivities $\varepsilon_j$ (in our notation). Medium 1 occupies the $z < 0$ half-space and medium 2 the $z > 0$; the graphene sheet is located at the $z = 0$ plane. Source: ref. [29].
FIG. 15: Spectrum of TM GSPPs in tBLG with θ = 9°: dependency on the Fermi level/carrier density. The black dots in (a) mark the fixed parameter in (b). The frequency, f, is given by \( f = \omega/(2\pi) \).

FIG. 16: Spectrum of TM GSPPs in tBLG with θ = 1.8°: dependency on the Fermi level/carrier density. The black dots in (a) mark the fixed parameter in (b). The frequency, f, is given by \( f = \omega/(2\pi) \).

In figs. 15–16, we present an analysis for two different twist angles. For θ = 9°, we see that the “signatures” of the curves do not differ a lot from those of the SLG [29] (which we also have computed as benchmark). This happens due to two main reasons: 1) within the SLG [29] (which we also have computed as benchmark), the curves \( n(\theta, \mu) \) are also very close (see fig. 10b). For θ = 1.8°, the exact opposite occurs and it leads to the plot of fig. 16b which we highlight since it is totally distinct from all the results obtained before. As an immediate application, we can think of using these results as an alternative method for determining θ.

V. CONCLUSIONS AND FUTURE WORK

In this work, besides the understanding of the most recent models for the tBLG, we introduced a new method and improved to compute the Drude weight —eq. (6). In addition, original results for the plasmonic response of this system were achieved (see figs. 15–16 with emphasis for fig. 16b). Nevertheless, a more extensive study on the behavior of these curves with the variation of θ remains to be done, in order to investigate more promising applications. We leave for future work the study of the transverse electric (TE) modes, which are the ones that, in contrast to the TM modes, exist only when \( \theta < 90° \). The transverse electric modes are the ones that, in contrast to the TM modes, exist only when \( \theta < 90° \).

Finally, since this is an extended abstract of a master’s dissertation, it is worth mentioning that, here, due to the limitations in the number of pages, we did not tackle one of the chapters of the thesis, which concerns the effects of electron-electron interactions (an absent topic in literature for the tBLG), in particular the self-energy correction for the band renormalization due to the long range (screened) Coulomb repulsion. Although we were not able to compute the self-energy corrections yet, we provided a discussion on the difficulties encountered and strategies to solve them in future works.

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