Optical Hall response of bilayer graphene: the manifestation of chiral hybridized states in broken mirror symmetry lattices

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Abstract. Understanding mechanisms governing the optical activity of layered-stacked materials is crucial for designing devices aimed to manipulate light at the nanoscale. Here, we show that both the twisted and slid bilayer graphene are chiral systems able to deflect the polarization of the linear polarized light. However, only the twisted bilayer graphene supports the circular dichroism. Our calculation scheme, based on the time-dependent Schrödinger equation, is specifically efficient for calculating the optical-conductivity tensor. In particular, it allows us showing the chirality of hybridized states as the handedness-dependent bending of the trajectory of kicked Gaussian wave packets in the bilayer lattices. We show that the nonzero Hall conductivity is the result of the non-cancelling manifestation of hybridized states in chiral lattices. We also demonstrate the continuous dependence of the conductivity tensor on the twist angle and the sliding vector.
1. Introduction

Stacked two-dimensional (2D) materials represent a unique platform for the manipulation of light at the nanometer scale, therefore, representing an ideal platform aiming to advance for future emerging technologies [1, 2, 3, 4]. Additionally, twisted stacks of graphene or other so-called 2D van-der-Waals materials may realize twistronics and optoelectronics devices based on tuning their electronic structure [5, 6, 7, 8, 9, 10, 11, 12]. It was predicted that using the Bernal-stacked bilayer graphene may produce a finite Faraday rotation of light when travelling through a microcavities [13]. In recent experiments, it was demonstrated twisted bilayer graphene (TBG) can be used of manipulating the polarization state of light, resulting in a finite circular dichroisms (CD) [14]. Since intrinsic monolayer graphene does not have this property, understanding how twisting layers of graphene results in a finite optical activity, besides being a fundamental physical question is also essential for the development of nanodevices with novel chiral properties [14] with important applications for recognizing different enantiomers of molecules [15, 16].

Usually, the application of a magnetic field leads to the generation of a finite Faraday and Kerr rotations of the light polarization plane [17, 18, 19, 20]. However, it requires devices of large size, thus restricting their practical applications. It was found that electronic ground state with broken time-reversal symmetry (TRS) may support the appearance of Faraday rotation in the absence of a magnetic field [21, 22]. Strained graphene lattice was also shown to exhibit a giant Faraday and Kerr rotation [23, 24]. The electronic structure of strained graphene can be described by a picture of Weyl-like fermions moving in a gauge field [25, 26]. It was also pointed out that the physics of low-energy electronic states in TBG is governed by an effective non-Abelian gauge field [27, 28]. Similarly to spin-orbit interactions [29], these non-Abelian gauge fields preserve TRS [27]. An alternative analysis is terms of Berry curvature dipole has been recently proposed [30]. It has been predicted that the deformation of electron states caused by twisting and sliding graphene layers will manifest themselves through unique transport and optical properties such as a nonzero optical Hall response and the anisotropy of the longitudinal conductance [31, 32, 33, 34, 35].

Phenomenological models are usually employed for describing the optical activity of solids, see Refs. [36, 37, 35] for recent proposals describing the low-frequency regime of the chiral response in chiral 2D materials. However, a microscopic approach has been recently proposed by Suárez Morell et al. in Ref. [38]. Here, the analysis of the optical activity is based on the decomposition of the current operator into components in each graphene layer. They introduced an external parameter describing the phase factor characterizing the dephasing of the currents in two different graphene layers. The optical Hall conductivity is then deduced as the result of the correlation between the current components in the two layers. They concluded that the relative rotation of the electron chirality due to the lattice twisting and the current dephasing are the origin for the circular dichroism of the TBG system.
In this work, we present a microscopic analysis for the optical activity of TBG. We find that decomposing the current into the different contributions from the two layers is not a conclusive interpretation for describing the optical activity of TBGs and the other bilayer graphene (BLG) systems [38]. Instead, we notice a crucial role played by the electron dynamics in the twisted or slid lattices. Under twisting or sliding, the change of the lattice symmetry induces the spatial deformation of the wave functions of hybridized electron states. It is thus responsible for the chiral response of the bilayer graphene systems. We introduce as first an efficient scheme to calculate for all elements of the optical conductivity tensor rather than only the longitudinal conductivities. Our approach allows considering the electron dynamics at the atomic scale and respecting all-natural symmetries of the atomic lattice [39]. Secondly, we show how the optical Hall response of the system is governed not only by the inter-layer current-current correlations as pointed out by Suárez Morell et al., but by the intra-layer current-current correlations as well.

In the following, we show that only hybridized states formed by electrons between the two layers govern the optical activity of the bilayer system. These hybridized states support the electron propagation not only in each graphene layer but also interchangeably between the two layers [40, 41]. However, their contribution to the Hall response depends on their spatial symmetries. We show that when the mirror symmetry is broken, the hybridized states have no cancelling contribution to the optical Hall conductivity, resulting in a nonzero value for this quantity. Our analyses are based on a real-space approach, entirely at the microscopical level. To study the optical Hall response, we express the Kubo formula for the conductivity tensor in the form of the Kubo-Bastin formula. On a practical level, we obtain the conductivity tensor within the Kernel Polynomial Method (KPM) [42, 43, 44, 41]. This numerical approach allows us working with arbitrary configurations of the bilayer graphene, i.e., taking into account both the twist angle and the sliding vector, and respecting all-natural symmetries of the bilayer atomic lattice. We do not need to find the electronic eigenfunctions explicitly: we performed the calculation based on the analysis of the time-evolution of two kinds of states in the bilayer lattice — the localized $2p_z$-states and the kicked Gaussian wave packets. We show that the trajectory of the centroid of wave packets deviate from the direction of the initial wave vector and, the deviated direction depends on the initial layer location of the wave packet. This demonstrates the transverse correlation of the electron motion and hence, the dependence of the Hall response on the chirality of the bilayer lattice.

The paper is organized as follows: in Sec. 2, we present a model used to describe the dynamics of electrons in the BLG lattice together with the Kubo-Bastin formula. In Sec. 3, we discuss the optical Hall response of the BLG configurations through the analysis of the behaviour of the optical conductivity components. In Sec. 4 we present results illustrating the wave-packet dynamics in single layer and BLG systems. We devote Sec. 5 to discuss the optical activity of the BLG system through the determination of the Faraday and Kerr rotation angles as well as the circular dichroism. Finally,
our conclusions are given in the last section, Sec. 6. A few technical appendices are completing the manuscript: in Appendix A we give details on the Kubo-Bastin formula for the conductivity tensor and its evaluation in terms of the KPM. In Appendix B, we provide a highlight of the representation of relevant operators in terms of Chebyshev polynomials. In Appendix C we highlight the relation between the components of the conductivity tensor and optical coefficients.

2. Model and method

To characterise the dynamics of electrons in the BLG system we use a microscopic approach based on a tight-binding Hamiltonian describing electrons in the $2p_z$ orbitals of carbon atoms. The system Hamiltonian reads [45, 46, 43, 41, 44]:

$$\hat{H} = \sum_{\nu=1}^{2} \sum_{i,j} t_{ij}^{\nu} |i\rangle \langle j| + \sum_{\nu \neq \nu' = 1}^{2} \sum_{ij} t_{ij}^{\nu \nu'} |\nu i\rangle \langle \nu' j|.$$  

(1)

Here, the first term defines the dynamics of electron in each of the monolayer labeled by the index $\nu$ from site $i$ to site $j$ with the intra-layer hopping energy $t_{ij}^{\nu}$; the basis set is given by the ket-states $\{|\nu i\rangle\}$ representing the $2p_z$-orbitals of carbon atoms. The second term in Eq. (1) describes the electron hopping between two layers which is characterized by the hopping parameters $t_{ij}^{\nu \nu'}$. We use the Slater-Koster formalism to determine the values of the hopping parameters $t_{ij}^{\nu}$ and $t_{ij}^{\nu \nu'}$ [45, 46, 41]. In this work, we will ignore effects of the graphene sheet curvature [47, 48, 49]; we assume the spacing between the two layers constant and about $d \approx 3.35$ Å and set all onsite energies to be zero. We will treat the BLG system in the general form by considering two different types of configurations: (a) twisted bilayer graphene, and (b) slid bilayer graphene (SBG). In the case (a), the two layers are rotated with respect to each other by a twist angle $\theta$. In general, in this configuration the system does not have translational symmetry, but supports moiré patterns — a typical feature of TBG configurations. The translational symmetry is only recovered for a discrete, but infinite set of twist angles given by the expression:

$$\cos \theta = \frac{3q^2 - p^2}{3q^2 + p^2},$$

where $p$ and $q$ are integers [50]. When the twist angle $\theta$ satisfies this equation, the staking of two monolayer lattices is called commensurate, otherwise incommensurate. The unit cell of commensurate TBG configurations with tiny twist angles usually contains thousands of carbon atoms, causing limitations in the calculation using exact diagonalization procedures. In contrast, in the configuration (b), translational symmetry is preserved, but the point group symmetries are changed compared to the case without sliding. The unit cell is always defined in this configuration and it is composed of 4 carbon atoms, two from each layer [32, 27].

The key to theoretically study the Hall response of an electronic system is to calculate and analyze the electrical conductivity tensor. In linear response theory, there
are several formulations for the Kubo conductivity suitable for calculating either the longitudinal conductivities or the transversal ones [51, 52, 53, 54]. Starting from a real-space approach, we aim to calculate all the elements of the conductivity tensor within a unique formalism that also works for systems lacking translational invariance [55, 56, 43]. Specifically, we use the following expression to calculate the conductivity tensor, also known as Kubo-Bastin formula [57, 56]:

$$\sigma_{\alpha\beta}(\omega) = \frac{ie^2}{\omega} \int_{-\infty}^{+\infty} dEf(E) \text{Tr} \left\{ \delta(E - \hat{H}) \hat{v}_\alpha \hat{G}^+(E + \hbar \omega) \hat{v}_\beta \\ + \hat{G}^-(E - \hbar \omega) \hat{v}_\alpha \delta(E - \hat{H}) \hat{v}_\beta \right\}, \quad (2)$$

where $\hat{G}^\pm(E) = (E - \hat{H} \pm i\delta)^{-1}$ are the retarded (+) and advanced (−) resolvents, respectively, and $\hat{v}_\alpha = i [\hat{H}, \hat{x}_\alpha]/\hbar$ is the $\alpha$-component of the velocity operator.

In Appendix A, we present the derivation for Eq. (2) starting from the more general Kubo formula. We implement Eq. (2) within the KPM by using the Chebyshev polynomials of the first kind, $T_m(x) = \cos[m \arccos(x)]$, to represent the operators:

$$\delta(E - \hat{H}) = \frac{\theta(1 - \epsilon)\theta(1 + \epsilon)}{W\sqrt{1 - \epsilon^2}} \sum_{m=0}^{\infty} \frac{2}{\delta_{m,0} + 1} T_m(\epsilon) T_m(\hat{h}), \quad (3)$$

$$\hat{G}^\pm(E) = \frac{1}{W} \sum_{m=0}^{\infty} \frac{2}{\delta_{m,0} + 1} (\mp i)^{m+1} g_m^\pm(\epsilon \pm i\eta) T_m(\hat{h}). \quad (4)$$

In the previous expressions, we have rescaled the energy variable and the Hamiltonian in the range of $(-1, 1)$:

$$E \rightarrow \epsilon = \frac{E - E_0}{W} \quad \hat{H} \rightarrow \hat{h} = \frac{\hat{H} - E_0}{W},$$

where $W$ is the half of spectrum bandwidth, $E_0$ is the central point of the spectrum. The function $g_m(z)$ is defined by

$$g_m^\pm(z) = \frac{1}{\sqrt{1 - z^2}} \left( \sqrt{1 - z^2} \pm iz \right)^m \quad (5)$$

with complex variable $z$ taking the values as $z_\pm = \epsilon \pm i\eta$ to define the resolvents $\hat{G}^\pm$.

Substituting expressions (3) into Eq. (2) leads to calculate the so-called Chebyshev momenta

$$\chi_{mn} = \text{Tr}[T_m(\hat{h}) \hat{v}_\alpha T_n(\hat{h}) \hat{v}_\beta]. \quad (6)$$

These quantities are commonly evaluated by stochastic methods with the use of a set of random phase states [42]. In our work, we use the scheme of randomly sampling the basis set to build a small set of $|\nu\rangle$ [43, 41]. When adopting this set of states, the Chebyshev momenta $\chi_{mn}$ are simply evaluated by $\chi_{mn} = \sum_i \chi^{(i)}_{mn}$ where $\chi^{(i)}_{mn} = \langle \nu \mid T_m(\hat{h}) \hat{v}_\alpha T_n(\hat{h}) \hat{v}_\beta \rangle \langle \nu \rangle$. One of the advantage of this technique is that it avoids special treatments of nodes near the sample edges, which are usually affected...
Optical Hall response of bilayer graphene

by boundary conditions imposed by calculation. Additionally, it allows to interpret the final result as the contribution of local information on each lattice site in particular domains of the lattice, e.g., the unit cell or the moiré cell in the TBG system.

3. Optical Hall response

We present in Fig. 1a) results of the optical conductivity tensors for four TBG configurations with the following twist angles \( \theta = 16.426^\circ, 11.635^\circ, 9.431^\circ \) and \( 3.890^\circ \). Though our numerical method allows to work with arbitrary values of the twist angle, these four values are chosen, close to the commensurate angles, to verify rigorously the symmetrical property of the conductivity tensor. We have verified the conductivity tensor has the following symmetry properties:

\[
\sigma_{xx}(\omega) = \sigma_{yy}(\omega),
\]

\[
\sigma_{xy}(\omega) = -\sigma_{yx}(\omega) \neq 0.
\]

Additionally, the value of these elements are independent of the reference frame fixed for the calculation. In Fig. 1b) we show the optical conductivity tensors for several SBG configurations with different sliding vectors \( \tau \) with the length \( \ell_{\tau} = 0.8a_{cc}, 0.6a_{cc}, 0.4a_{cc}, 0.2a_{cc} \) and the angle \( \phi_{\tau} = 12^\circ \) here \( a_{cc} \approx 0.145 \) nm is the nearest distance between two carbon atoms in the graphene monolayer. For SBGs, since the translational symmetry of the lattices is preserved, we calculated the optical conductivity tensor using the two methods: the Kubo-Bastin formula in the real-space approach and the Kubo-Greenwood formula in the reciprocal lattice space approach (see Appendix A). For the latter case, we express the conductivity tensor as

\[
\sigma_{\alpha\beta}(\omega) = \sum_{k \in \text{BZ}} \sigma_{\alpha\beta}(k, \omega),
\]

where the vector \( k \) is defined in the first Brillouin zone (BZ). We verified that results from the two methods coincide. For SBGs, we found in general that conductivity tensor has the following symmetry properties:

\[
\sigma_{xx}(\omega) \neq \sigma_{yy}(\omega),
\]

\[
\sigma_{xy}(\omega) = \sigma_{yx}(\omega).
\]

It means that the SBG is optically anisotropic. The symmetry property is different from the case of TBGs in Eqs. (7). Additionally, the specific values of the conductivity tensor components depend on the choice of the Cartesian axes. However, the values for the conductivity tensor in two different Cartesian frames are related by the standard coordinate transformation \( \sigma'(\omega) = R_{\varphi}\sigma(\omega)R_{\varphi}^{-1} \), where \( R_{\varphi} \) is the \( 2 \times 2 \) rotation matrix transforming one frame to the other. In particularly, we found that in the cases that the sliding vector \( \tau \) is either collinear or perpendicular to one of the vectors \( \delta_i \) with \( i = 1, 2, 3 \), i.e. the vectors connecting one carbon atoms to its three nearest neighbors in the honeycomb lattice, the optical Hall conductivity \( \sigma_{xy}(\omega) \) is zero in the reference frame with \( \tau \) collinear with the \( Ox \) axis. These results for TBGs and SBGs are completely
different from those for the AA- and AB-stacked configurations where the conductivity tensor is isotropic. In general, the appearance of a finite optical Hall conductivity, and the relations between the tensor components, are not related to the breaking of TRS, but to the spatial symmetries of the atomic lattices. For the bilayer system, the AA-stacking configuration presents the highest symmetry with the point group $D_{6h}$ and the space group $p6mm$. The symmetry of the AB-stacked configuration is lower with the point group $D_{3d}$ and the space group $p3m1$. Introducing a finite value of the twist angle $\theta$ and the sliding vector $\tau$ significantly reduces the symmetry of the resulted bilayer lattices. Specifically, $\theta$ breaks the translational and mirror symmetries, thus reducing the point group of the TBG lattices to be $D_6$ (or $D_3$ depending on the position of the twist axis) [39]. On the other hand, $\tau$ breaks all point group symmetries, but preserves the translational symmetry. However, when the sliding vector $\tau$ is collinear or perpendicular to one of the three vectors $\delta_i$, an axis $C_2'$ exchanging the two layers and a mirror plane perpendicular to this rotation axis is preserved. These elements, together with an inversion center $I$, form the point group $C_{2h}$. Within these symmetry considerations, we verify that both the TBG and SBG lattices are chiral. In fact,
the TBG configurations with the twist angles of $\theta$ and $-\theta$ are the mirror images of each other, but never coincident. Similarly, the SBG configurations with $\mathbf{\tau} = (\tau_x, \tau_y)$ and $\mathbf{\tau}' = (\tau_x, -\tau_y)$ are also the mirror images of each other and never identical if the lattice has no the mirror symmetry. Such point groups of the TBG and SBG lattices are given in the three-dimensional space. However, because of the 2D nature, the physical properties of these systems are governed by the 2D sub-groups of these ones, i.e., $C_s$ for SBGs and $C_6$ (or $C_3$) for TBGs. Thus, it is easy to verify that $\sigma_{xx} = \sigma_{yy}$ and $\sigma_{yx} = -\sigma_{xy}$ for TBGs and $\sigma_{xy} = \sigma_{yx}$ and $\sigma_{xx} \neq \sigma_{yy}$ for SBGs, confirming the data we have obtained numerically. The vanishing of $\sigma_{xy}(\omega)$ in special bilayer configurations, as the SBG ones with the $C_{2h}$ symmetrical point group and also the AA- and AB-stacked configurations, is clearly due to the cancelling contribution of optical transitions enforced by the mirror symmetry. Indeed, because of the preservation of a mirror plane in the SBGs with $\mathbf{\tau} \propto \mathbf{\delta}_i$, the Hamiltonian is even with respect to $k_y$, i.e., $\hat{H}(k_x, k_y) = \hat{H}(k_x, -k_y)$ but the electric current component $\hat{j}_y$ is odd since $\hat{v}_y(k_x, k_y) = (1/\hbar)\partial \hat{H}(k_x, k_y)/\partial k_y$. As a consequence, the quantity $\sigma_{xy}(k_x, k_y)$ becomes odd with respect to $k_y$, i.e., $\sigma_{xy}(k_x, k_y) = -\sigma_{xy}(k_x, -k_y)$. As a result, the contribution from all Bloch states in the first BZ will mutually cancel leading to $\sigma_{xy}(\omega) = 0$. For TBGs, the interpretation of its optical activity is more subtle: Suárez Morell et al. addressed it in terms of the rotation of the isospin of the graphene Weyl fermions [38]. However, this is not sufficient because if the two graphene layers are decoupled, the behaviour of the system must be identical to that of the monolayer, i.e., with $\sigma_{xy}(\omega) = 0$. We can show that by decreasing the interlayer hopping parameter $t_\perp$, the longitudinal conductivity of TBGs approaches to the value of twice the conductivity of monolayer graphene, and the Hall conductivity vanishes as seen in Figs. 2a) and 2b). Following Suárez Morell et al., we also decomposed the electron velocity operator $\hat{v}_\alpha$ into the terms involving the electron motion in each graphene layer, the in-plane or intra-layer velocities $\hat{v}_\alpha^{(1)}$, and the inter-layer velocities $\hat{v}_\alpha^{(2)}$, i.e., $\hat{v}_\alpha = \hat{v}_\alpha^{(1)} + \hat{v}_\alpha^{(2)} + \hat{v}_\alpha^{(12)}$. By denoting
The optical Hall conductivity $\sigma_{xy}(\omega)$ (the red solid curve) as the result of the correlation of various terms of the total velocity operators $\hat{v}_\alpha = \sum_\mu \hat{v}_\mu^\alpha$, $\mu = 1, 2, 12$. Here $\sigma_{xy}^{\mu\nu}(\omega) \propto \langle \hat{v}_\mu^\nu(\omega) \hat{v}_\nu^\mu \rangle$. The data is presented for a SBG lattice with $\tau = (1.5a_{cc}, 12^\circ)$. The terms corresponding to the correlation of the interlayer current $\hat{v}_{12}$ are small and not shown.

$\langle \hat{v}_\mu^\nu(\omega) \hat{v}_\nu^\mu \rangle$ the velocity-velocity correlation functions, according to the linear-response theory, we can assign the optical Hall conductivity $\sigma_{xy}^{\mu\nu}(\omega)$ to $\sigma_{xy}^{\mu\nu}(\omega) = ie^2 \langle \hat{v}_\mu^\nu(\omega) \hat{v}_\nu^\mu \rangle / \omega$. Here we denote $\mu, \nu$ the indices for the electron velocity terms, which take the value $\mu, \nu = 1, 2, 12$. From the Hamiltonian (2) these velocity terms are determined by:

$$\hat{v}_\nu^\mu = \frac{i}{\hbar} \sum_{i,j} t_{ij}^{\nu \mu} (\mathbf{r}_j^\nu - \mathbf{r}_i^\nu) |\nu i\rangle \langle \nu j| \ \nu = \{1, 2\}, \quad (11)$$

$$\hat{v}_{12} = \frac{i}{\hbar} \sum_{\nu \neq \mu=1}^2 \sum_{i,j} t_{ij}^\nu (\mathbf{r}_j^\nu - \mathbf{r}_i^\nu) |\nu i\rangle \langle \nu j|, \quad (12)$$

the latter can be further simplified by decomposing $\mathbf{r}_j^2 - \mathbf{r}_i^1 = \mathbf{d}_{GG} + \mathbf{r}_{ij}$, i.e. into a vertical and a horizontal contribution, respectively. Here $\mathbf{d}_{GG}$ is the vector vertically connecting the two graphene layers with the length $d_{GG} = 0.335$ nm. The velocity in Eq. (12), can be therefore expressed as the sum of two perpendicular contributions $\hat{v}_{12}^z = \hat{v}_{12}^z + \hat{v}_{12}^{\text{drag}}$. Since $\hat{v}_{12}^{\text{drag}}$ lies in the lattice plane, only this component contributes to the velocity-velocity correlator.

In Fig. 3 we display data for a SBG configuration with the sliding vector $\tau = (1.5a_{cc}, 12^\circ)$. We see that the magnitude of $\sigma_{xy}^{11}(\omega)$ and $\sigma_{xy}^{22}(\omega)$ are comparable to that of $\sigma_{xy}^{12}(\omega)$ and $\sigma_{xy}^{21}(\omega)$, while that of $\sigma_{xy}^{12}(\omega)$ and $\sigma_{xy}^{21}(\omega)$ are negligible and not shown. These data indicate clearly that the appearance of the optical Hall conductivity is not dictated solely by the correlation of the electron velocities in two different graphene layers, but by the correlation of the velocities in the same graphene layer as well. A different explanation was proposed by Kim et al. in Ref. [14], they stated that the circular dichroism of TBGs is due to the interlayer optical transitions. However, the interlayer optical transitions occur as well in the AA- and AB-stacked configurations but $\sigma_{xy}(\omega) = 0$. All these analyses suggest that we need to pay particular attention to
determine the essential factors governing the optical transitions, and hence, the velocity-velocity correlation: the electronic states conducting the current. Unfortunately, it is merely impossible to visualize these states. However, in the following, we will present a way to analyze their behavior through the dynamics of wave packets.

4. Wave-packet dynamics

To unveil the physics of the optical Hall response, we numerically tracked the time evolution of electrons in the TBG lattices. In Fig. 4 we display a snapshot at time 2.9 fs of the distribution of the probability density of electron initially occupying a single $2p_z$ orbital in layer 1. We observed that the electron wave does not spread solely in layer 1, but it penetrates and spreads into layer 2 as well. The electron wave propagation is always interchangeable between the two layers. It implies the existence of hybridized states that supports such a wave interchange. Noticeably, the wavefronts of the electron waves in two layers present differences and similarities: both wavefronts show the anisotropy of the wave spreading along the six preferable directions parallel to the zigzag lines of the honeycomb lattice [41]. However, the relative rotation of the two lattices, it shows the misalignment of the preferable directions of electron propagation in the layer 2 compared to the layer 1. This result partially supports the conclusion by Suárez Morell et al. in Ref. [38]. To clarify the key role played by the hybridized states in governing the finite Hall conductivity, we investigated the evolution of kicked Gaussian waves

$$\psi(r, t = 0) \propto \exp \left[ -\frac{(r - r_0)^2}{4\xi^2} \right] \exp( iqr), \quad (13)$$

where $r_0$ is the initial center of the wave packet, $\xi$ is its width and $q$ the initial wave
As a first, we tracked the trajectory of the wave centroid in the lattice of monolayer graphene. The wave centroid at time $t$ is defined by the vector

$$
\mathbf{r}_c(t) = \sum_i \mathbf{r}_i |\psi(\mathbf{r}_i, t)|^2
$$

(14)

where the summation is over all lattice nodes $\mathbf{r}_i$. We observed that the wave centroid always evolves along straight lines parallel to the direction of the initial wave vector $\mathbf{q}$ independently of the zigzag and armchair directions of the honeycomb lattice — see Fig. 5a). Semi-classically, it implies that an electron injected into the honeycomb lattice with an initial velocity $\mathbf{v}_q(0) \propto \mathbf{q}$ will move along this direction without any deflection, i.e., $\mathbf{v}_q(t) \propto \mathbf{q}$ at time $t > 0$. Denoting with $v_{q\parallel}$ and $v_{q\perp}$ the components of the velocity $\mathbf{v}_q$ of the wave centroid parallel and perpendicular to $\mathbf{q}$, respectively, we have $v_{q\parallel} = v_{q\parallel}$ and $v_{q\perp} = 0$. It yields $\langle v_{q\parallel}(\omega)v_{q\parallel} \rangle = 0$. Since $\sigma_{xy}(\omega)$ can be regarded as the result of the average of the velocity-velocity correlation functions over all possible values of $\mathbf{q}$ and $\mathbf{r}_0$, i.e., $\sigma_{xy}(\omega) \propto \langle v_{q\parallel}(\omega)v_{q\parallel} \rangle$, it therefore explains why the zero optical Hall conductivity of monolayer graphene. We note in passing that the same argument applies for the case of AA-stacked bilayer graphene. However, for the AB-stacked lattice, we observed the oscillation behavior of the wave centroid trajectories along the six preferable directions of the electron propagation — see Fig. 5b). By decreasing the interlayer hopping parameter $t_{\perp}$, the oscillation amplitude of the trajectories reduces. The oscillation trajectories are a peculiar feature of the hybridized electron states in the AB-stacked lattice. Remember that in this atomic lattice, three $\sigma_v$ mirror planes of the honeycomb lattice are broken, but replaced by three $C'_2$ axes that interchange the two graphene layers. The motion of electron is thus not constrained by the mirror symmetry, but by the $C'_2$ symmetry. More importantly, the oscillation trajectories indicate that electron gains a nonzero transverse velocity $v_{q\perp} \neq 0$ when moving in the lattice, leading to $\langle v_{q\parallel}(\omega)v_{q\parallel} \rangle \neq 0$. However, analysing in details Fig. 5b) we can infer the zero Hall conductivity $\sigma_{xy}(\omega) = 0$ by noticing that there are always two mirror symmetric trajectories related by the symmetry plane $\sigma_d$ of the AB-stacked lattice corresponding to two distinct values of $\mathbf{q}$. We note in passing that a similar behaviour is also observed for the particular SBG configurations with the $C_{2h}$ symmetry. This suggests that the existence of a mirror symmetry plane in the bilayer lattices will always lead to the existence of pairs of momenta $\mathbf{q}$ and $\mathbf{q}'$ such that $v_{q\parallel}' = -v_{q\parallel}$, but $v_{q\perp}' = v_{q\perp}$. As a consequence, these terms always cancel each other on average, resulting in the zero optical Hall conductivity, i.e., $\sigma_{xy}(\omega) = 0$. In Fig. 5c) we show the trajectories of the wave centroid of kicked Gaussian wavepackets in a TBG lattice. The solid (dashed) curves are for the cases that the initial wave packets locate in layer 1 (layer 2). We clearly see the deflection of the trajectories from the lines along the initial vector $\mathbf{q}$, it means that $\langle v_{q\parallel}(\omega)v_{q\parallel} \rangle \neq 0$. Because of the absence of the mirror symmetry, the TBG lattices are chiral. It dictates as well the chirality of the hybridized electron states as the mirror images of the solid and dashed curves shown in Fig. 5c). A further study of the centroids of the wave parts propagating on two graphene layers shows that they moves along the different curly trajectories — see Fig. 5d). It explains why the deflection of the
trajectories and the left-, right-deflection (chirality) behaviours observed in Fig. 5c). So, with the same argument made for the monolayer and AB-stacked bilayer we conclude that the TBG lattices will be characterized by a finite optical Hall conductivity since there are no cancellation contributions to \( \langle v_{q\perp}(\omega)v_{q\parallel} \rangle \) in the optical Hall conductivity due to the breaking of the mirror symmetry, i.e., \( \sigma_{xy}(\omega) \propto \langle v_{q\perp}(\omega)v_{q\parallel} \rangle \neq 0 \) after averaging over \( \mathbf{q} \) and \( \mathbf{r}_0 \).

5. Faraday, Kerr rotation and Circular dichroism

In the previous section we have seen that the electrical conductivity tensor is the key quantity to characterize the transport and optical properties of an electronic system. To complete our discussion, we present in here results for the Faraday and Kerr rotation...
The Optical Hall response of bilayer graphene

Figure 6. (a) The Faraday $\theta_F$ and Kerr $\theta_K$ rotation angles and (b) the circular dichroism as a function of the photon energy for a representative TBG configuration with the twist angle $\theta = 9.430^\circ$ versus the photon energy. The plot of the CD is shifted upward an amount of 2.5 and data is multiplied by 20 to compare with $\sigma_{xx}$. The CD is displayed (the red curve) together with the real part of the conductivity $\sigma_{xx}/\sigma_0$ (the blue curve) to associate the structure of the former with that of the conductivity. (c) The DOS as a function of the energy for TBG with $\theta = 9.430^\circ$ in red. The DOS of the totally decoupled BLG (in blue) is also displayed to highlight the energy ranges in which the hybridized states are manifested through the sub-peaks of the red curve.

angles of the light polarization vector as well as the CD, a quantity quantifying the difference of the absorption of the left-handed and right-handed circular polarization light. We employed the transfer matrix method to determine the transmission $t$ and reflection $r$ matrices; these express the relationship between the amplitude of the transmitted/reflected light and that of the incident light [22]. The details of calculation are presented in Appendix C where the relationship between these matrices and the components of the electrical conductivity tensor is presented. In particular, we show that $t_{xy}(\omega), r_{xy}(\omega) \propto \sigma_{xy}(\omega)$, see Eqs. (C.24) and (C.25). From these results, together with Eqs. (C.17) and (C.12), we see that there are no Faraday and Kerr rotation as well as the CD if the systems do not have the Hall response, $\sigma_{xy}(\omega) \neq 0$. For the case of SBG systems, because of the specific symmetry properties of the conductivity tensor, i.e., $\sigma_{xy}(\omega) = \sigma_{yx}(\omega)$, Eq. (C.31) indicates that there is no the CD. In other words, the SBG systems cannot distinguish the left-handed and right-handed circular polarized light despite the chirality of the atomic lattice. It is different from the case of TBG systems since $\sigma_{xy}(\omega) = -\sigma_{yx}(\omega)$. In Fig. 6a) and Fig. 6b) we present the values of the Faraday, Kerr rotation angles and of the CD calculated for a TBG configuration with the twist angle $\theta = 9.430^\circ$ (The results for the other twist angles are qualitatively similar).

These results show that these quantities vary versus the photon energy $\omega$ of the incident light. In the low ($< 1$ eV) and high ($> 7$ eV) energy ranges wherein the electronic states in two graphene layers effectively decouple, the values of $\theta_F, \theta_K$ and the CD are zero as expected. On the contrary, in the energy range of (1, 7) eV where...
the hybridized electron states are formed and manifest as the peaks in the density of states [43], the values of $\theta_K$, $\theta_F$ and CD are different from zero. For the TBG configuration with $\theta = 9.430^\circ$ we observe that $\theta_F$ can reach the value of $4^\circ$, $\theta_K$ of $2^\circ$, and the CD of $\sim 8\%$. In general, the dependence of these quantities on the photon energy $\omega$ is complicated an it is presented in Eq. (C.31). Physically, since the CD associates to the light absorption, the behavior of the curve CD($\omega$) should relate to the real part of the longitudinal conductivities $\sigma_{xx}(\omega)$ and $\sigma_{yy}(\omega)$. In Fig. 6b) we present the curve CD($\omega$) together with the curve $\sigma_{xx}(\omega)$ in which the CD values are multiplied by 20 times and shifted upward an amount of 2.5 as a guide for the eyes. Clearly, we observe the consistency of the behavior of the CD($\omega$) result with that of the conductivity curve $\sigma_{xx}(\omega)$.

6. Discussion and conclusions

Before concluding the paper we would like to validate available predictions of physical properties of generic TBG systems that were usually deduced for commensurate configurations. As our calculation method is based on the real-space approach, it can be applied to lattices of arbitrary stacking, regardless of commensurate or incommensurate configuration. Using our numerical method, we can conclude that both the density of states and the conductivity tensor $\sigma$ continuously vary with the twist angle $\theta$ and the sliding vector $\tau$ in the whole range of these parameters, i.e., $\theta \in (0^\circ, 60^\circ)$ and $\tau$ given in the triangle defined by two unit vectors $a_1$ and $a_2$ of the honeycomb lattice. However, it is worth noticing that the behaviours of the AA- and AB-stacked configurations cannot be deduced as limiting cases of the TBG system for $\theta \to 0^\circ$ or $60^\circ$ or of the SBG system for $\tau \to 0$. We confirm this argument by a symmetry analysis: as long as $\theta \neq 0$ or $60^\circ$ or $\tau \neq 0$ the system symmetries are not changed by varying these parameters. A sudden change is obtained only when either $\theta$ or $\tau$ are equal to the limit values. For these cases, the point group $D_6$ (or $D_3$) of the TBG lattices changes to $D_{6h}$ (or to $D_{3d}$) of the AA-stacked lattice (or of the AB-stacked lattice), whereas for the case of SBG, the change is from $E$ to $C_s$ or to higher symmetry point groups. Additionally, for the TBG case, there will be a collapse of the unit cell from the very large size to the one containing only 4 carbon atoms when $\theta$ changes to $0$ or $60^\circ$. In both the AA- and AB-stacked lattices, the number of carbon atoms in one layer is coupled to another one in the second layer is higher than that in the TBG and SBG lattices. Indeed, by defining $\bar{n}_{nb}$ the average number of lattice nodes on one layer that electron can hop from another node in the other layer: for a given radius of proximity $r_c = \sqrt{a_{cc}^2 + d^2}$, we find it is $\bar{n}_{nb} = 4(5)$ for $\theta = 0^\circ(60^\circ)$, but $\bar{n}_{nb} \approx 2.7$ for different values of $\theta$, no matter how the small of $\theta$. This observation is interesting because it can help to explain the behaviour of effective decoupling of the two layers in some energy ranges [58, 43].

In conclusion, stacking material layers of atomic thickness has been considered as a potential path for engineering the electronic structure and physical properties of complex 2D material systems, especially aiming to design devices for manipulating light
at the nanoscale [59, 4]. This can be of potential interest for designing optical systems able to distinguish different enantiomers of molecules with important application in medicine and chemistry [15, 16, 60]. In this work, we analyzed in-depth the origin of the finite optical Hall response of bilayer graphene under twisting and/or sliding relatively two layers. We showed that the lattices of twisted- and slid-bilayer graphene are chiral and support the ability of rotating the polarization of the linearly polarized light. Our analysis was based on a real-space computation scheme developed to compute all components of the optical conductivity tensor. We showed in detail that the TBG lattices are isotropic and support the CD, and the SBG lattices are anisotropic and do not support the CD. The calculation method allows us to monitor the evolution of electron in the atomic bilayer lattices with arbitrary twist angle and sliding vector. The chiral behavior of the hybridized electron states was Figure out as the deflection of the trajectory of the kicked Gaussian wave packets in the BLG lattices. The optical Hall response of the BLG system was therefore argued as the manifestation of the chirality of the hybridized states that supports the interchange of electrons between the two graphene layers. However, we shown that the mirror symmetry constrains the contribution of such states to the optical Hall response. In the lattices without the mirror symmetry like TBGs and SBGs, the hybridized states govern the correlation of different components of the electron velocity in a way that terms do not cancel each other, hence resulting in the nonzero optical Hall conductivity. To quantify the optical activity of the bilayer graphene systems we employed the transfer matrix method to establish the relations of the transmission and reflection matrices to the components of the conductivity tensors and then determined the Faraday and Kerr rotation angles as well as the circular dichroism. Finally, taking the advantage of the calculation method, combined with a symmetry analysis, we concluded the continuous variation of physical quantities, including the density of states and the electrical conductivity tensors, on the twist angle and the sliding vector. This conclusion is a basis to generalize knowledge of bilayer graphene systems that would be deduced using the force-brute exact diagonalization approach.

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Appendix A. The Kubo-Bastin formula

There are a number of versions of the Kubo formula for the electrical conductivity suitable for implementing it in different situations. Here we present the derivation
for Eq. (2.) From the general linear response theory, the element $\sigma_{\alpha\beta}(\omega)$ of the electrical conductivity tensor is composed of the diamagnetic and paramagnetic parts, $\sigma_{\alpha\beta}(\omega) = \sigma^A_{\alpha\beta}(\omega) + \sigma^P_{\alpha\beta}(\omega)$ in which [61]:

$$\sigma^A_{\alpha\beta}(\omega) = \frac{i e^2}{m_e \omega} n_e \delta_{\alpha\beta},$$ \hspace{1cm} (A.1)

$$\sigma^P_{\alpha\beta}(\omega) = \frac{i e^2}{\omega} \sum_{\ell,n} \left( f_n - f_{\ell} \right) \frac{\langle n | \hat{v}_\alpha | \ell \rangle \langle \ell | \hat{v}_\beta | n \rangle}{\hbar(\omega + i\eta) - (E_\ell - E_n)}$$ \hspace{1cm} (A.2)

Here $m_e$ is the bare electron mass, $n_e$ the electron density in a system, $\eta$ a positive infinitesimal number, and $\Omega$ the spatial volume of the considered system. The diamagnetic part is diagonal. It is determined through the calculation of $n_e$:

$$n_e = \int_{-\infty}^{+\infty} dE \rho(E) f(E) = \int_{-\infty}^{+\infty} dE \frac{\rho(E)}{1 + e^{\beta(E - \mu)}},$$ \hspace{1cm} (A.3)

where $\rho(E)$ is the density of states of electron, $\beta = 1/k_B T$ the inversion of thermal energy, and $\mu$ the chemical potential. For the paramagnetic part of the conductivity elements $\sigma^P_{\alpha\beta}(\omega)$, by taking the properties of the delta-Dirac function involving the integration they are written as follows:

$$\sigma^P_{\alpha\beta}(\omega) = \frac{i e^2}{\omega} \sum_{\ell,n} \int_{-\infty}^{+\infty} dE \delta(E - E_n) f(E) \frac{\langle n | \hat{v}_\alpha | \ell \rangle \langle \ell | \hat{v}_\beta | n \rangle}{E + \hbar \omega - E_\ell + i\eta},$$

$$+ \frac{i e^2}{\omega} \sum_{\ell,n} \int_{-\infty}^{+\infty} dE \delta(E - E_\ell) f(E) \frac{\langle n | \hat{v}_\alpha | \ell \rangle \langle \ell | \hat{v}_\beta | n \rangle}{E - \hbar \omega - E_n - i\eta}. \hspace{1cm} (A.4)$$

Now with the notice that $\delta(E - \hat{H}) | n \rangle = \delta(E - E_n) | n \rangle$ and introducing the retarded $(\theta)$ and advanced $(-)$ resolvents:

$$\hat{G}^\pm(E \pm i\omega) = \frac{1}{E \pm (\hbar \omega + i\delta) - \hat{H}}.$$ \hspace{1cm} (A.5)

Equation (A.4) is written in the form of Eq. (2):

$$\sigma^P_{\alpha\beta}(\omega) = \frac{i e^2}{\omega} \int_{-\infty}^{+\infty} dE f(E) \text{Tr} \left[ \delta(E - \hat{H}) \hat{v}_\alpha \hat{G}^+(E + i\omega) \hat{v}_\beta \right]$$ \hspace{1cm} (A.6)

$$+ \hat{G}^-(E - i\omega) \hat{v}_\alpha \delta(E - \hat{H}) \hat{v}_\beta$$ \hspace{1cm} (A.7)

For low frequencies we can approximate

$$\hat{G}^\pm(E \pm i\omega) \approx \hat{G}^\pm(E) \pm \frac{d\hat{G}^\pm(E)}{dE} \hbar \omega.$$ \hspace{1cm} (A.8)

So, we determine the real and imaginary parts of the conductivity $\sigma^P_{\alpha\beta}$ as follows

$$\text{Re}[\sigma^P_{\alpha\beta}(\omega)] = -\frac{e^2 \hbar}{\Omega} \int_{-\infty}^{+\infty} dE f(E) 2\text{Im} \left[ \text{Tr} \left[ \delta(E - \hat{H}) \hat{v}_\alpha \frac{d\hat{G}^+(E)}{dE} \hat{v}_\beta \right] \right],$$ \hspace{1cm} (A.9)

$$\text{Im}[\sigma^P_{\alpha\beta}(\omega)] = +\frac{e^2}{\Omega \omega} \int_{-\infty}^{+\infty} dE f(E) 2\text{Re} \left[ \text{Tr} \left[ \delta(E - \hat{H}) \hat{v}_\alpha \hat{G}^+(E) \hat{v}_\beta \right] \right].$$ \hspace{1cm} (A.10)

The imaginary part is inversely dependent on $\omega$ but the real part is independent of $\omega$. The real part is identical to the Kubo-Bastin formula that defines the dc
Optical Hall response of bilayer graphene

conductivity [57]. As the delta-function and Green functions can be expanded efficiently in terms of Chebyshev polynomials, i.e., with the expansion coefficients given analytically, the Kubo-Bastin formula is useful for general calculation. In Ref. [56] the authors demonstrated successfully the calculation for the dc conductivity of topological systems.

Appendix B. Retarded and advanced resolvents in terms of Chebyshev polynomials

The Bessel function of the first kind is defined by the integral:

$$J_n(z) = \frac{1}{\pi i} \int_0^\pi d\theta \cos(n\theta) e^{iz \cos \theta}.$$  \hspace{1cm} (B.1)

This function has the property: $$J_n(-z) = (-1)^n J_n(z).$$

In terms of the Chebyshev polynomials of the first kind, it is straightforward to expand the exponent function $$e^{\pm ixt}$$. It yields

$$e^{\pm ixt} = \sum_{n=0}^{+\infty} 2 \delta_{n,0} + 1 (\pm i)^n J_n(t) T_n(x).$$  \hspace{1cm} (B.2)

where $$x \in (-1, 1)$$.

Apply this result to expand the retarded and advanced resolvents $$\hat{G}^\pm(E) = 1/(E \pm i\eta - \hat{H}) = W^{-1}/(\epsilon \pm i\eta - \hat{h})$$, where $$\epsilon = (E - E_0)/W, \hat{h} = (\hat{H} - E_0)/W$$, we have:

$$\hat{G}^\pm(E) = \pm \frac{1}{W} \sum_{n=0}^{+\infty} (\mp i)^{n+1} \frac{2}{\delta_{n,0} + 1} g^\pm_n(\epsilon \pm i\eta) T_n(\hat{h})$$  \hspace{1cm} (B.3)

where $$g^\pm_n(\epsilon \pm i\eta)$$ are defined by: [54]

$$g^\pm_n(z) = \int_0^{+\infty} dt e^{\pm izt} J_n(t) = \frac{(\sqrt{1-z^2} \pm iz)^n}{\sqrt{1-z^2}}.$$  \hspace{1cm} (B.4)

where $$z = \epsilon \pm i\eta$$.

The derivative of the resolvents $$\hat{G}^\pm(E)$$ with respect to $$E$$ is driven as follows:

$$\frac{\partial \hat{G}^\pm(E)}{\partial E} = \pm \frac{1}{W} \sum_{n=0}^{+\infty} (\mp i)^{n+1} \frac{2}{\delta_{n,0} + 1} \frac{\partial g^\pm_n(\epsilon \pm i\eta)}{\partial E} T_n(\hat{h})$$

$$= \pm \frac{1}{W^2} \sum_{n=0}^{+\infty} (\mp i)^{n+1} \frac{2}{\delta_{n,0} + 1} \frac{\partial g^\pm_n(z)}{\partial z} T_n(\hat{h}),$$

where $$z = \epsilon \pm i\eta$$ and

$$\frac{\partial g^\pm_n(z)}{\partial z} = \frac{1}{\sqrt{1-z^2}} \left( \frac{z}{\sqrt{1-z^2}} \pm in \right) g^\pm_n(z).$$  \hspace{1cm} (B.5)
Optical Hall response of bilayer graphene

Appendix C. Faraday, Kerr rotation and circular dichroism

Appendix C.1. Elliptical polarization light

A monochromatic light is described by an electric vector with the components given in the form:

\[ E_x(t, z) = E_{0x} \cos(kz - \omega t) \quad (C.1) \]
\[ E_y(t, z) = E_{0y} \cos(kz - \omega t + \varphi) \quad (C.2) \]

where \( \varphi \) is the dephasing between the two components \( E_y \) and \( E_x \). This light is elliptically polarized and is characterized by two parameters, i.e., the polarization angle \( \alpha \) and the ellipticity \( \tan \epsilon \) (\( \epsilon \) is called the ellipticity angle). These two parameters are straightforwardly determined by:

\[ \tan(2\alpha) = \frac{2E_{0x}E_{0y}}{E_{0y}^2 - E_{0x}^2} \cos \varphi, \quad (C.3) \]
\[ \tan \epsilon = \left| \frac{E_{0x} \tan \alpha + E_{0y}}{E_{0x} - E_{0y} \tan \alpha} \right| \quad (C.4) \]

where \( \alpha \in (-\pi/4, \pi/4) \) and \( \epsilon \in [0, \pi/2) \).

In practice, we usually use a complex field to represent a trigonometric function. We thus define a complex vector, named the Jone vector, for the electric field as follows:

\[ E = \frac{1}{\sqrt{E_{0x}^2 + E_{0y}^2}} (E)_{0x} \quad E_y = \frac{1}{\sqrt{E_{0x}^2 + E_{0y}^2}} (E)_{0y} e^{i\varphi}. \quad (C.5) \]

So, a monochromatic light of the vertical and horizontal linear polarization (\( \varphi = 0 \)) is defined by the following Jone vectors:

\[ \tilde{E}_v^\ell = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{and} \quad \tilde{E}_h^\ell = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (C.6) \]

Similarly, for the left-handed (\( \varphi = \pi/2 \)) and right-handed (\( \varphi = -\pi/2 \)) circular polarization light they are defined respectively by the Jone vectors:

\[ \tilde{E}_L^c = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} \quad \text{and} \quad \tilde{E}_R^c = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}. \quad (C.7) \]

In general, for the left-handed (\( \varphi = \pi/2 \)) and right-handed (\( \varphi = -\pi/2 \)) elliptical polarization light in the canonical frame (\( \alpha = 0 \)) the Jone vectors read:

\[ \tilde{E}_L^e = \begin{pmatrix} \cos \epsilon \\ i \sin \epsilon \end{pmatrix} \quad \text{and} \quad \tilde{E}_R^e = \begin{pmatrix} \cos \epsilon \\ -i \sin \epsilon \end{pmatrix}. \quad (C.8) \]

Appendix C.2. Equations for the polarization angle and the ellipticity

Given a monochromatic light of the linear polarization parallel to the \( Oz \) axis. This light is incident to a plane separating two material environments. The lights transmitting and reflecting at this plane will be defined by Eqs. (C.1) and (C.2). Accordingly, the
Faraday and Kerr rotation angles are determined by the value of the polarization angle $\alpha$.

Using the complex representation for the components of the electric vector of a monochromatic light the polarization angle $\alpha$ and the ellipticity $\tan \epsilon$ are not determined by Eqs. (C.3) and (C.4). Instead, we define the complex quantity:

$$\chi = \frac{\tilde{E}_y}{\tilde{E}_x} = \frac{E_{0y}}{E_{0x}} e^{i\phi}. \quad (C.9)$$

Since in the canonical frame of the ellipse the Jones vector of the electric field is given by Eq. (C.8), we should rotate it back by an angle of $\alpha$ to obtain the vector components in the global Cartesian frame $xOy$. We therefore obtain:

$$\begin{pmatrix} \tilde{E}_x \\ \tilde{E}_y \end{pmatrix} = \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} \cos \epsilon \\ i\eta \sin \epsilon \end{pmatrix} \quad (C.10)$$

where $\eta = \pm 1$ is the sign for the left-handed and right-handed elliptical polarization. The quantity $\chi$ is thus determined by

$$\chi_{\eta} = \tan \alpha + i\eta \tan \epsilon \quad (C.11)$$

From this result it is straightforward to deduce the equations for the polarization angle and the ellipticity angle:

$$\tan(2\alpha_{\eta}) = \frac{2 \text{Re}(\chi_{\eta})}{1 - |\chi_{\eta}|^2}, \quad (C.12)$$

$$\sin(2\epsilon_{\eta}) = \eta \frac{2 \text{Im}(\chi_{\eta})}{1 + |\chi_{\eta}|^2}. \quad (C.13)$$

Now applying these results to determine the Kerr and Faraday rotation angles occurring at one reflection plane. In the given setup the Jones vector for the incident light is:

$$\tilde{E}^{\text{in}} = \begin{pmatrix} \tilde{E}_x^{\text{in}} \\ 0 \end{pmatrix}. \quad (C.14)$$

The Jones vectors for the reflecting and transmitting lights relate to $\tilde{E}^{\text{in}}$ through the reflection and transmission matrices $r$ and $t$, respectively, by $\tilde{E}^r = r \tilde{E}^{\text{in}}$ and $\tilde{E}^t = t \tilde{E}^{\text{in}}$. In particular,

$$\begin{align*}
\tilde{E}_x^r &= r_{xx} \tilde{E}_x^{\text{in}}, & \tilde{E}_y^r &= r_{yx} \tilde{E}_y^{\text{in}}, \\
\tilde{E}_x^t &= t_{xx} \tilde{E}_x^{\text{in}}, & \tilde{E}_y^t &= t_{yx} \tilde{E}_y^{\text{in}}. \quad (C.15)
\end{align*}$$

where $r_{\alpha\beta}$ and $t_{\alpha\beta}$ are the elements of the matrices $r$ and $t$. We thus obtain the expression for the $\chi$-quantity as follows:

$$\chi_K = \frac{\tilde{E}_y}{\tilde{E}_x} = \frac{r_{yx}}{r_{xx}} \quad \text{and} \quad \chi_F = \frac{\tilde{E}_y}{\tilde{E}_x} = \frac{t_{yx}}{t_{xx}}. \quad (C.17)$$

Plugin $\chi_K$ and $\chi_F$ into Eq. (C.12) we obtain the Kerr and Faraday rotation angles $\theta_K, \theta_F$. 
Appendix C.3. Relations between the transmission and reflection matrices to the electrical conductivity tensor

We follow the transfer matrix method to establish the expression for the transmission and reflection matrices for the system of bilayer graphene. We set up the system like the one in Ref. [22] in which the graphene layer separating two semi-infinite mediums 1 and 2 characterized by the parameters \((\epsilon_1, \mu_1)\) and \((\epsilon_2, \mu_2)\). Ignoring the thickness of the graphene layer we can assume that the interface between the two mediums has an electrical conductivity tensor \(\tilde{\sigma} = \sigma_0 \sigma\). The boundary conditions for the Maxwell equations at the interface therefore read:

\[
\tilde{E}^{\text{in}} + \tilde{E}^r = \tilde{E}^t \tag{C.18}
\]

\[
n \times (\tilde{H}^t - \tilde{H}^{\text{in}} - \tilde{H}^r) = \tilde{J} \tag{C.19}
\]

Here \(n\) is the normal vector of the interface and \(\tilde{J}\) is the electrical current density on the interface. Because of the Ohm’s law

\[
\tilde{J} = \tilde{\sigma} \tilde{E}^t = \tilde{\sigma} (\tilde{E}^{\text{in}} + \tilde{E}^r), \tag{C.20}
\]

and the relation

\[
\tilde{H} = \sqrt{\frac{\epsilon_0 \epsilon}{\mu_0 \mu}} k \times \tilde{E} \tag{C.21}
\]

we identify the expression for the transmission matrix [34]:

\[
t = 2 \sqrt{\frac{\epsilon_0 \epsilon_1}{\mu_0 \mu_1}} \left[ \left( \sqrt{\frac{\epsilon_0 \epsilon_1}{\mu_0 \mu_1}} + \sqrt{\frac{\epsilon_0 \epsilon_1}{\mu_0 \mu_1}} \right) I + \tilde{\sigma} \right]^{-1}. \tag{C.22}
\]

Here \(I\) is the identity matrix. The reflection matrix \(r\) is determined via the relation \(r + t = I\).

Assume \(\mu_1 = \mu_2 = 1\) and note the definition of the refractive index \(n_{1,2} = \sqrt{\epsilon_{1,2}}\) we have:

\[
t = 2 \left[ (1 + n_{21}) I + \tilde{\sigma} \right]^{-1}. \tag{C.23}
\]

where \(n_{21} = n_2/n_1\), \(\tilde{\sigma} = (4\pi\alpha/n_1 e^2)\tilde{\sigma} = (\pi\alpha/n_1)\sigma\) and \(\alpha = e^2/(4\pi\hbar c) \approx 1/137\) is the fine-structure constant. Proceeding with further calculations we obtain:

\[
t = \frac{2}{\Delta} \begin{pmatrix}
1 + n_{12} + \tilde{\sigma}_{yy} & -\tilde{\sigma}_{xy} \\
-\tilde{\sigma}_{yx} & 1 + n_{12} + \tilde{\sigma}_{xx}
\end{pmatrix} \tag{C.24}
\]

and

\[
r = \frac{2}{\Delta} \begin{pmatrix}
1 + n_{12} + \tilde{\sigma}_{yy} - \frac{\Delta}{2} & -\tilde{\sigma}_{xy} \\
-\tilde{\sigma}_{yx} & 1 + n_{12} + \tilde{\sigma}_{xx} - \frac{\Delta}{2}
\end{pmatrix} \tag{C.25}
\]

where \(\Delta = [(1 + n_{21}) + \tilde{\sigma}_{xx}] [(1 + n_{21}) + \tilde{\sigma}_{yy}] - \tilde{\sigma}_{xy}\tilde{\sigma}_{yx}\).
Appendix C.4. Circular dichroism

The circular dichroism is a quantity used to measure the dependence of the light absorption on the left-handed and right-handed polarization:

$$CD = \frac{A_L - A_R}{A_L + A_R},$$  \hspace{1cm} (C.26)

where $A_{L/R}$ are the absorptances. These quantities are determined through the reflectance $R$ and transmittance $T$ by $A_{L/R} = 1 - (R_{L/R} + T_{L/R})$. Here the reflectance and transmittance are determined by

$$R = \frac{(\mathbf{r}^{in})^\dagger (\mathbf{r}^{in})}{(|\mathbf{E}^{in}|)^2},$$  \hspace{1cm} (C.27)

$$T = \frac{(\mathbf{t}^{in})^\dagger (\mathbf{t}^{in})}{(|\mathbf{E}^{in}|)^2}.$$  \hspace{1cm} (C.28)

In particular, with the notice of the Jones vector given in Eq. (C.7) the absorptance of the left/right-handed circular light are given by:

$$A_L = \text{Re} \left[ t_{xx} + i(t_{xy} - t_{yx}) + t_{yy} \right],$$  \hspace{1cm} (C.29)

$$A_R = \text{Re} \left[ t_{xx} - i(t_{xy} - t_{yx}) + t_{yy} \right].$$  \hspace{1cm} (C.30)

The formula for the CD therefore reads:

$$CD = \frac{\text{Im}(\bar{\sigma}_{xy} - \bar{\sigma}_{yx})}{\text{Re}[2(1 + n_{21}) + \bar{\sigma}_{xx} + \bar{\sigma}_{yy}]}.$$  \hspace{1cm} (C.31)

For mediums 1 and 2 being vacuum, we can set $n_1 = n_2 = n_{21} = 1$.

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