Angular momentum anisotropy of Dirac carriers: A new twist in graphene

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Dirac carriers in graphene are commonly characterized by a pseudospin degree of freedom, arising from the degeneracy of the two inequivalent sublattices. The inherent chirality of the quasiparticles leads to a topologically non-trivial band structure, where the in-plane component of sublattice spin and momentum are intertwined. Equivalently, sublattice imbalance is intimately connected with angular momentum, inducing a torque of opposite sign at each Dirac point. In this work we develop an intuitive picture that associates sublattice spin and winding number with angular momentum. We develop a microscopic perturbative model to obtain the finite angular momentum contributions along the main crystallographic directions. Our results can be employed to determine the angular dependence of the $g$-factor and of light absorption in honeycomb bipartite structures.

\section{I. INTRODUCTION}

The linear dispersion at the Fermi level of graphene is cognate with the Dirac cones of massless relativistic particles \cite{1}, motivating extensive research towards the parallelism with relativistic quantum mechanics and quantum electrodynamics (QED) in solid-state materials \cite{2–8}. In this Dirac-like model, the notion of sublattice (SL) spin plays the role of real spin, with ‘up’ and ‘down’ states being associated with the two SL components that constitute the honeycomb structure. The inherent chirality of the Dirac carriers leads to a topologically non-trivial band structure, where the related edge’s helicity gives rise to the spin-Hall insulator \cite{9–11}. The presence of a pseudospin degree of freedom in the Hamiltonian allows a parallelism between its torque and that of the angular momentum \cite{12, 13}, where an experimental connection has been realized only in photonic graphene \cite{14–16}.

In this work we evaluate the constants of motion and provide an intuitive connection between SL spin and angular momentum in the neighborhood of the Fermi energy. We develop a microscopic perturbative model to obtain the corrections to the angular momentum $\hat{L}$ in terms of atomic parameters. We consider band hybridization, spin-orbit coupling (SOC) and Bychkov-Rashba effect, and obtain a peculiar anisotropy in the corrections, owing to the relation of $\hat{L}$ and SL spin. These corrections have been verified in large graphene samples, by measuring the $g$-factor corrections \cite{17}.

This manuscript is organized as follows: First we employ symmetry arguments to analyze the low-lying quasiparticle Hamiltonian. We examine perturbatively the $d$-orbital contribution to the $\pi$-bands ($l = 2$, $m_l = \pm 1$), and calculate the correction to the angular momentum. Finally, we include perturbatively the mixing with the $\sigma$-band ($l = 1$, $m_l = \pm 1$) via atomic SOC and Bychkov-Rashba interaction, and obtain the angular momentum corrections in terms of atomic parameters.

\section{II. BAND MIXING AND HYBRIDIZATION}

A. Dirac electrons to lowest order: $\langle \hat{L} \rangle = 0$ orbitals

Dirac electrons near the Fermi edge are commonly described by $\pi$-orbitals within a nearest neighbors (NN) tight-binding model \cite{18, 19}. The two sublattices that constitute the honeycomb structure lead to two energy bands, whose interplay yields a conical quasiparticle spectrum. The concept of isospin or SL spin is commonly introduced, where the $z$-component, $\sigma_z$, accounts for the SL occupation imbalance. At the Dirac points (DPs), the quasiparticle Dirac-like Hamiltonian reads $\langle 9, 12, 18, 19 \rangle$:

$$\hat{H}_0 = \hbar v_F (\tau q_x \hat{\sigma}_x + q_y \hat{\sigma}_y) + \lambda \hat{\sigma}_z = \hbar v_F \hat{\mathbf{q}} \cdot \hat{\mathbf{\sigma}} + \lambda \hat{\sigma}_z,$$

where we have assigned the valley index $\tau = 1$ and $\tau = -1$, respectively, to the DPs, $K$ and $K'$, and $\hat{\mathbf{q}} = (q_x, q_y)$ is the small vector off the nearest DP. Here, $v_F \approx 10^6$ m s$^{-1}$ is the Fermi velocity, $s_n$, $\hat{\sigma}_n$ are the Pauli matrices representing the electron spin and sublattice-spin, respectively, and we have defined the vector $\hat{\mathbf{\sigma}}_\tau \equiv (\tau \hat{\sigma}_x, \hat{\sigma}_y)$. The first term originates from the quantum mechanical hopping between the two sublattices and tends to align $\hat{\mathbf{q}}$ and $\hat{\mathbf{\sigma}}_z$. In spite of involving the Pauli matrices, it is a \textit{scalar} (see Appendix A). The second term can be, however, a scalar, in the case of a Kane-Mele SOC \cite{9} ($\lambda \hat{\sigma}_z = \tau \lambda \hat{s}_z \hat{\sigma}_z$) or a pseudoscalar, in case of Semenov insulator \cite{20}, $\lambda \hat{\sigma}_z = \varepsilon_{AB} \hat{\sigma}_z = (\varepsilon_A - \varepsilon_B) \hat{\sigma}_z/2$, owing to the broken parity symmetry. The distinction is important, as it is only in the latter case where a direct analogy with the equations of a dipole in a magnetic field can be made.

To lowest order, the eigenenergies of (1) are given by:

$$\varepsilon_{\pm} = \pm \sqrt{(\hbar v_F |q|)^2 + \lambda^2}.$$

The corresponding eigenstates are commonly given in terms of the dominant ($p_z$-orbital) contribution to sublattices $A$ and $B$ for $q \neq 0$,

$$|\varphi_{\pm}^{(0)}\rangle \approx c_A |p_z^A\rangle + c_B |p_z^B\rangle,$$

where $c_A / c_B = \pm e^{i\tau \varphi_q}$, $\varphi_q = \arctan q_y / q_z$.

\vspace{1em}

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The relative phase between the two sublattice components \( \tau \phi_q \) results indeed in a Berry phase [21], and determines the direction of the associated SL spin [22, 23], in analogy with chirality and charge conjugation in QED [2, 5]. At the critical point \( q = 0 \), however, the SL spin components are decoupled, and the solutions depend on the (pseudo) scalar nature of the mass term. A scalar, Kane-Mele SOC results in decoupled bispinors where the conduction band in \( K \) relates to the valence band in \( K' \), leading to the spin-Hall effect [9, 10]. On the other hand, the Semenov term results in a trivial insulator, with the peculiarity of pseudoscalar eigenvalues at the DPs, in analogy with a dipole in a magnetic field.

We evaluate now the expectation value of the SL spin components. For the states of (3), we obtain:

\[
\sigma^0 \equiv \langle \varphi_\pm^{(0)} | \sigma_z | \varphi_\pm^{(0)} \rangle = |c_A|^2 - |c_B|^2,
\]

\[
\langle \hat{\sigma}_\tau^\parallel \rangle^0 \equiv \left( \langle \tau \hat{\sigma}_x \rangle, \langle \tau \hat{\sigma}_y \rangle \right) = \pm \left( \tau \cos \varphi_q \tau, \tau \sin \varphi_q \tau \right) = \pm \left( q_x, q_y \right),
\]

where we have used \( 2|c_A|^2 \approx 1 \). A three-component axial vector \( \hat{\sigma}_\tau \), was already identified with the real angular momentum [12, 13]. Doing so, however, results in unphysical interpretations for the equations of motion or the conserved quantities, owing to the different physical meaning of the different components. Here we aim at bringing clarity and physical meaning to the connection between the angular momentum components \( \hat{L}_\parallel, \hat{L}_z \), and \( \hat{\sigma}_\parallel, \sigma_z \). For the easy-axis, the \( z \)-component of angular momentum is associated with the pseudoscalar \( \tau \sigma_z \):

\[
\hat{H}_0, \hat{L}_z = -\frac{\hbar}{2} \left[ \hat{H}_0, \hat{\sigma}_z \right] = -i\hbar v_F \hat{\sigma}_\parallel ^\parallel \times \hat{p} = -i\hbar \hat{r} \times \hat{p},
\]

where we have used that \( \hat{r} = (i/\hbar) [\hat{H}_0, \hat{n}] = v_F \hat{\sigma}_\tau \), that is, \( \hat{\sigma}_\parallel ^\parallel \) is aligned with the velocity [13]. As Mecklenburg et al. already pointed out [12], this implies that the constant of motion is \( 2L_z + \hbar \sigma_z \), which we generalize to bilayer graphene’s Dirac Hamiltonians in terms of the winding number \( \nu \) (see Appendix B) as:

\[
\frac{d}{dt} (2L_z + \nu \hbar \tau \sigma_z) = 0.
\]

That means that sublattice imbalance induces a torque in the quasiparticle spectrum of opposite sign on each valley. Likewise, a finite \( L_z \) induces a sublattice imbalance of opposite sign on each valley. The same line of argument can be used in the presence of a Kane-Mele term, where \( \langle \tau \sigma_z \rangle \) has different sign for electrons with opposite spin, resulting in splitting of left- or right-propagating states [9, 24]. This peculiarity is reflected in the band mixing, as will be detailed in the next section: Dirac electrons on a given SL (say \( A \)) and valley couple only to clockwise rotating orbitals, and the converse is true for those on SL \( B \).

An intuitive picture can be given in terms of the winding number: in mono- (bi-)layer graphene, the Berry phase is \( \pi (2\pi) \), yielding a \( \nu = 1 \) (2) winding number. This means that an adiabatic closed contour in momentum space the SL spin ‘winds’ around the origin once (twice), just like momentum does [25]. This rotational in momentum space can then be intuitively associated with a torque, and hence, its path integral should be related to the angular momentum.

For the in-plane components we may define an in-plane pseudovector operator

\[
\hat{\mathcal{L}}_\parallel = (\hat{\lambda}/\hbar) \hat{p} \times \hat{u}_z,
\]

that could relate to in-plane angular momentum. With this definition, we obtain:

\[
\frac{d}{dt} \hat{\mathcal{L}}_\parallel = \frac{i}{\hbar} \left[ \hat{H}_0, \hat{\mathcal{L}}_\parallel \right] = -\hat{\lambda} \left( -\hat{\sigma}_y \hat{\tau} \right) = \hat{\lambda} \hat{\sigma}_\parallel ^\parallel \times \hat{u}_z.
\]

On the other hand, we may calculate \( \hat{\sigma}_\parallel \) as:

\[
\frac{1}{v_F} \frac{d}{dt} \hat{r} = \frac{1}{\hbar} \frac{d}{dt} \hat{\sigma}_\parallel = \frac{i}{\hbar} \left[ \hat{H}_0, \hat{\sigma}_\parallel \right] = -2v_F \tau \left( -\hat{q}_y \hat{q}_x \right) \hat{\sigma}_z + \hat{\lambda} \left( -\hat{\sigma}_y \hat{\tau} \right),
\]

that is, together with (7), we obtain the in-plane relation,

\[
\frac{d}{dt} \left( \frac{\hat{\mathcal{L}}_\parallel + \hat{\lambda} \hat{\sigma}_\parallel ^\parallel}{2} \right) = \hbar v_F \tau \left( -\hat{q}_y \hat{q}_x \right) \hat{\sigma}_z.
\]

This implies that \( 2\hat{\mathcal{L}}_\parallel + \hbar \hat{\sigma}_\parallel ^\parallel \) is a constant of motion as long as SL symmetry is preserved, \( \sigma^0 = 0 \) or strictly at the DPs, if the Hamiltonian contains a non-zero mass term. To lowest order, using (4) in (9), we obtain:

\[
\frac{d}{dt} \hat{\mathcal{L}}_\parallel \left( 1 - \hbar v_F q \lambda^{-1} \hat{\sigma}_z \right) + \frac{\hbar}{2} \frac{\hat{\sigma}_\parallel ^\parallel}{dt} = 0,
\]

Note that the second term in the brackets evaluates to zero in the absence of a mass term, \( \lambda = 0 \). Although \( \hat{\sigma}_z \) can be associated with \( \hat{L}_z \), no connection exists for the in-plane counterparts, however, we can relate \( \hat{\sigma}_\parallel \) to \( \hat{\mathcal{L}}_\parallel \) at DPs, which is beyond the scope of this work.

On what follows, we focus on the different angular momentum components and their relation to sublattice imbalance. We note that neither a Semenov term nor a Kane-Mele term provides a valley-sublattice imbalance, as \( \langle \tau \sigma_z \rangle = 0 \) when averaging over the low-lying energy states. Indeed, the axial symmetry of the \( p_x \) orbitals, with \( l = 1 \) and \( m_l = 0 \), involves \( \langle L_m \rangle = 0 \), \( \alpha = x, y, z \). However, (i) band hybridization and band mixing, (ii) atomic spin orbit coupling, (iii) Bychkov-Rashba effect and (iv) structural spin-orbit coupling may finite contributions to the angular momentum. We consider in the following sections these general mixing mechanisms from a microscopic perspective, and provide an intuitive connection with SL-spin degree of freedom.
B. The hybridized \( \pi \)-bands

We consider the \( \pi \)-band hybridization near the DPs, which is, to lowest order, given by \( p_z \) orbitals of Eq. (3). Using perturbation theory within the two-center Slater-Koster approximation, the contributions from the \( d \)-band are obtained via hopping to \( d_{xy} \) and \( d_{xz} \) orbitals, [26, 27] (see also Appendix C):

\[
|\varphi_d^{(1)}\rangle = \frac{3i\tau V_{pd\pi}}{\sqrt{2}\varepsilon_{pd}} \left( c_A|2\tau\rangle^B + c_B|2 - \tau\rangle^A \right),
\]

where \( \varepsilon_{pd} \) is the energy of the \( d \)-relative to the \( p \)-orbitals, with \( \varepsilon_d \gg \varepsilon_p \), justifying our perturbative approach and we have employed the angular momentum representation, \( |2 \pm 1\rangle = (|d_{xz}\rangle \mp i|d_{yz}\rangle)/\sqrt{2} \). It is straightforward to see that the expectation value of the in-plane angular momentum is still zero, \( \langle \hat{L}_{\pi} \rangle_{\pi} = \langle \hat{L}_{\pi} \rangle_{\tau} = 0 \). We note, however, that within our NN model, the \( p_z \) orbital in \( A \) sublattice couples to \( |2\tau\rangle^B \), which is a clockwise rotating \( B \) for \( \tau = 1 \) (at point) and to the anti-clockwise rotating \( B \) in \( K' \), allowing us to associate SL spin and \( L_z \) in an intuitive manner. Using (10), we have:

\[
\langle \hat{L}_{\pi} \rangle_{\pi} = \langle \varphi_d^{(1)}|\hat{L}_{\pi}|\varphi_d^{(1)}\rangle = \left( \frac{3V_{pd\pi}}{\sqrt{2}\varepsilon_{pd}} \right)^2 \tau \sigma_0^z \sim \frac{\lambda_I}{\lambda_{soc}} \tau \sigma_0^z,
\]

where in the last step we have used the result of Konschuh et al. [26]. Fig. 1a. illustrates, in essence, the spin-valley-orbit coupling for the low-lying energy bands showing charge-conjugation, parity, time-reversal (CPT) symmetry. The conduction or electron band (CB) is characterized by \( \langle \tau s_z \sigma_z \rangle > 0 \). That is, a spin ‘up’ (‘down’) electron has \( \tau s_z > 0 \) ( \( \tau s_z < 0 \)), and hence, acquires a positive (negative) correction to the angular momentum (10), meaning a coupling to a counter-clockwise (clockwise) rotating \( d \) orbital. That is, the \( z \) component of the spin is aligned with the angular momentum correction. For the valence or hole band (VB), however, the converse occurs: having \( \tau s_z \sigma_z = -1 \), the spin anti-aligns with the angular momentum correction. The system is thus CPT-symmetric: For any left-handed electron state with positive energy \( \varepsilon_+ \), a corresponding conjugated right-handed hole state with energy \( \varepsilon_- = -\varepsilon_+ \) and opposite angular momentum can be found. The CPT symmetry and, ultimately, the chirality of Dirac electrons, is reflected in the proportionality to \( \tau \sigma_0^z \) of the angular momentum corrections.

C. The hybridized \( \sigma \)-bands

We consider next the hybridization of the \( \sigma \)-bands near the DPs. Once again, we employ the two-center Slater-Koster approximation for a \( s \)-orbital with \( p_{x,y} \) on its NN, at \( \vec{k} = \tau \vec{K} + \vec{q} \). Employing the angular momentum representation, \( |l, m_l\rangle \), and noting that \( |p_s\rangle = \mp i|p_d\rangle = \sqrt{2}|1 \pm 1\rangle \), the hybridized doublets (see Appendix D) are:

\[
\begin{align*}
|\phi_{A\pi}^+\rangle &= i\tau \cos\gamma|s^A\rangle + \sin\gamma|1\tau\rangle^B, \\
|\phi_{B\pi}^+\rangle &= i\tau \cos\gamma|s^B\rangle + \sin\gamma|1 - \tau\rangle^A, \\
|\phi_{A\pi}^-\rangle &= -i\tau \sin\gamma|s^A\rangle + \cos\gamma|1\tau\rangle^B, \\
|\phi_{B\pi}^-\rangle &= -i\tau \sin\gamma|s^B\rangle + \cos\gamma|1 - \tau\rangle^A, \\
|\phi_{AB}^0\rangle &= |1 - \tau\rangle^B, \quad |\phi_{BA}^0\rangle = |1\tau\rangle^A,
\end{align*}
\]

with corresponding eigenenergies:

\[
\varepsilon_{\sigma}^\pm = \frac{\varepsilon_s}{2} \pm \sqrt{\frac{\varepsilon_p^2}{4} + \frac{9\varepsilon_{soc}^2}{2}}, \quad \varepsilon_0 = 0.
\]

The \( p_z \)-orbitals described in (3) can mix with the \( \sigma \)-bands either intrinsically via atomic spin-orbit interaction or extrinsically, via e.g. Bychkov-Rashba effect [26–32]. The latter is linear in uniaxial field, and leads to the Stark effect, consisting of an atomic dipole moment induced by a perpendicular effective field, \( \vec{E} = E\hat{z} \). Microscopically, the induced dipole results in a non-zero intra-atomic coupling between the \( p_z \) and \( s \)-orbitals. The intrinsic SOC, on the other hand, couples the \( p_z \)-orbitals of the \( \pi \)-bands with the \( p_{x,y} \)-orbitals of the \( \sigma \)-bands.

The \( \sigma \)-band mixing near the Fermi energy is expected to be smaller than the \( d \) band contribution, since the spin-orbit coupling parameter and the Stark parameter, \( \lambda_z = eE(s|\hat{z}|p_z) \) are small compared to the \( p-d \) coupling, \( \lambda_{soc}^p, \lambda_z \ll V_{pd\pi} \). We thus consider the \( \sigma \) band mixing perturbatively on the following.

1. Atomic SOC of \( \sigma \) and \( \pi \) bands

We consider next the atomic SOC that mixes the \( p \)-orbitals, hence, coupling the \( \pi \) and \( \sigma \) bands:

\[
\hat{H}_{SOC} = i\lambda_{soc}^p \sum_{\alpha=A,B} \epsilon_{ijk} \delta_k |p_{j\alpha}\rangle \langle p_{j\alpha}| + \text{h.c.,}
\]
where $\lambda_{p_{\sigma}}$ is the spin-orbit coupling parameter for the $p$ orbitals and $\hat{s}_k$ is the $k$-Pauli matrix, acting on the spin degree of freedom. The action of $\hat{H}_{SOC}$ over the $p_{\sigma}$ orbitals ($\alpha = A, B$) is,

$$
\hat{H}_{SOC}[p_{\alpha}] \otimes |s_{z}| = \lambda_{p_{\sigma}} \sqrt{2}s_{z}|1-s_{z}|^\alpha,
$$

where the bar over the WF ($\bar{\phi}$) indicates opposite spin. The fist order correction to the $\pi$ orbitals of Eq. (3) is then:

$$
|\varphi^{(1)}_{\pi}| = \sum_{s,i} \langle \phi_{s,i}^{s} | \hat{H}_{SOC} | \varphi^{0}_s \rangle |\phi_{s,i}^{s}| = -\sqrt{2}c_A \hat{s}_z \lambda_{p_{\sigma}} \delta_{s_z,-\tau} \left[ \sin \frac{\gamma}{\varepsilon_\sigma} |\phi_{BA}^+\rangle + \cos \frac{\gamma}{\varepsilon_\sigma} |\phi_{BA}^-\rangle \right] -\sqrt{2}c_B \hat{s}_z \lambda_{p_{\sigma}} \delta_{s_z,\tau} \left[ \sin \frac{\gamma}{\varepsilon_\sigma} |\phi_{AB}^+\rangle + \cos \frac{\gamma}{\varepsilon_\sigma} |\phi_{AB}^-\rangle \right].
$$

Projecting over the terms that yield finite angular momentum correction, we obtain:

$$
\hat{\mathcal{P}}|\varphi^{(1)}_{\pi}| = \tau \alpha_{\pi} \left( c_A |1-\tau\rangle^A - c_B |1\tau\rangle^B \right),
$$

where we have defined the $\sigma$-band mixing coefficient,

$$
\alpha_{\pi} \equiv \sqrt{2} \lambda_{p_{\sigma}} \left( \sin^2 \frac{\gamma}{\varepsilon_\sigma} + \cos^2 \frac{\gamma}{\varepsilon_\sigma} \right).
$$

Formally, the correction given above is similar to that of (10), accounting for the chirality of the Dirac electrons. Employing the same arguments as in Sec. II B to Eq. (13), we conclude that spin 'up' electrons in the CB couple to a clockwise rotating $\sigma$ orbital, and the converse for spin 'down' electrons. CPT symmetry ensures that spin 'down' ('up') holes couple to (counter)-clockwise orbitals (see Fig. 1b).

2. Bychkov-Rashba SOC of $\pi$- and $\sigma$-bands

We can express the Bychkov-Rashba Hamiltonian microscopically as the coupling of the $p_z$ and $s$ orbitals,

$$
\hat{H}_{BR} = \lambda_z \hat{L}_z \sum_{\alpha=A,B} |s^{\alpha}\rangle |p_z^z\rangle + \text{h.c.},
$$

Since $\lambda_z$ is a very small energy scale, we can safely consider it small with respect to $\varepsilon_{\pm}$, and treat it perturbatively. The fist order correction to the $\pi$ orbitals of Eq. (3) is then:

$$
|\varphi^{(1)}_{\pi}| = -i\lambda_z c_A \hat{L}_z \left( \cos \frac{\gamma}{\varepsilon_\sigma} |\phi_{BA}^+\rangle - \sin \frac{\gamma}{\varepsilon_\sigma} |\phi_{BA}^-\rangle \right) + -i\lambda_z c_B \hat{L}_z \left( \cos \frac{\gamma}{\varepsilon_\sigma} |\phi_{AB}^+\rangle - \sin \frac{\gamma}{\varepsilon_\sigma} |\phi_{AB}^-\rangle \right).
$$

Using $\hat{L}_z = (\hat{L}_z s_z + \hat{L}_z s_{\tau})/2 + \hat{L}_z s_z$ and that $(\hat{L}_z s_z + \hat{L}_z s_{\tau})|1 \pm \tau\rangle = 2 \delta_{s_z,\tau} |p_z^z\rangle$, projecting onto the states with finite $m_1$, we obtain:

$$
\hat{\mathcal{P}}|\varphi^{(1)}_{\pi}| = -i\alpha_{\pi} \tau (c_A |1\tau\rangle^B \delta_{s_z,-\tau} + c_B |1-\tau\rangle^A \delta_{s_z,\tau}) + \text{h.c.},
$$

where we have defined:

$$
\alpha_{\pi} \equiv \lambda_z \left( \frac{1}{\varepsilon_\sigma} - \frac{1}{\varepsilon_{\pm}} \right) \sin \gamma \cos \gamma = \frac{\sqrt{2} \lambda_z}{3 V_{soc}}.
$$

3. Principal Plane Asymmetry Spin-Orbit Coupling

We consider, for completeness, a general spin-flipping next-NN SOC related to the absence of horizontal reflection [33, 34]. Although there is no terminological consensus, we adopt the acronym PIA, which can be used for pseudospin-inversion asymmetry [35] or more generally, for principal plane mirror asymmetry [35]. This term can be associated to the presence of ripples, defects or adsorbates, and it allows for a momentum-dependent coupling of the $p_z$ and $p_{x,y}$-orbitals, hence, allowing coupling between the $\pi$ and $\sigma$ bands. The orbital part of the coupling takes the general form $i\tau\beta$, with $\beta = 3n^p (V_{pp\sigma} - V_{pp\pi})/4$ real, as detailed in Appendix E:

$$
\hat{H}_{PIA} = i\tau \beta \left( |1\tau\rangle^B |p_z^z\rangle |\delta_{s_z,\tau}\rangle + |1-\tau\rangle^A |p_z^z\rangle |\delta_{s_z,-\tau}\rangle \right) + \text{h.c.}
$$

Near the DPs, we employ perturbation theory and obtain the correction due to PIA SOC:

$$
|\varphi^{(1)}_{\pi}| = \sum_{s,i} \langle \phi_{s,i}^{s} | \hat{H}_{SOC} | \varphi^{0}_s \rangle |\phi_{s,i}^{s}| = -i\tau \beta c_A \delta_{s_z,-\tau} \left[ \sin \frac{\gamma}{\varepsilon_\sigma} |\phi_{BA}^+\rangle + \cos \frac{\gamma}{\varepsilon_\sigma} |\phi_{BA}^-\rangle \right] -i\tau \beta c_B \delta_{s_z,\tau} \left[ \sin \frac{\gamma}{\varepsilon_\sigma} |\phi_{AB}^+\rangle + \cos \frac{\gamma}{\varepsilon_\sigma} |\phi_{AB}^-\rangle \right],
$$

which results, projecting over the relevant terms, on a first order correction similar to that of Bychkov-Rashba (14), only differing in the prefactor,

$$
\hat{\mathcal{P}}|\varphi^{(1)}_{\pi}| = i\tau \alpha_{\pi} \left( c_A |1\tau\rangle^B |\delta_{s_z,\tau}\rangle + c_B |1-\tau\rangle^A |\delta_{s_z,-\tau}\rangle \right) + \text{h.c.},
$$

with:

$$
\alpha_{\pi} = 3n^p (V_{pp\sigma} - V_{pp\pi}) \left( \frac{\sin^2 \gamma}{\varepsilon_\sigma} + \frac{\cos^2 \gamma}{\varepsilon_\sigma} \right).
$$

D. Angular momentum contribution of the $\sigma$ band

We first evaluate the in-plane corrections $\langle L_{x,y}\rangle/\sigma$, taking into account the first-order corrections due to atomic SOC given in (13). Using that $\sqrt{2}L_{x}|1,\pm\tau\rangle = |p_z^z\rangle$ and
\[ \sqrt{2} \hat{L}_y |1, \pm \tau \rangle \equiv \pm i \tau |p_d^\alpha \rangle, \] we notice that the only surviving first order correction is along the zig-zag direction:

\[ \langle \hat{L}_x \rangle_{\text{AT}} = 2 \Re\langle \varphi_\pm^{(0)} | \hat{L}_x | \varphi_{\text{AT}}^{(1)} \rangle = \pm 2 \sqrt{2} \alpha_{\text{AT}} \sigma_z^0, \]
\[ \langle \hat{L}_y \rangle_{\text{AT}} = 0, \] (17)

where the bar indicates that we have averaged over spin states. This in-plane anisotropy is due to the geometry of the lattice, with a propagating \( p_d \) orbital mode at the DPs. Recall that \( p_d \)-orbitals have a finite \( L_z \) contribution. The Bychkov-Rashba correction (14) and the PIA correction yield similar contributions:

\[ \frac{\langle \hat{L}_x \rangle_{\text{BR}}}{\langle \hat{L}_y \rangle_{\text{BR}}} = \mp 2 \sqrt{2} \alpha_{\text{BR}} \left( - \sin \varphi_q \cos \varphi_q \right), \] (18)

where we have used \( \langle \hat{L}_\alpha \rangle_{\text{BR}} = 2 \Re\langle \varphi_\pm^{(0)} | \hat{L}_\alpha | \varphi_{\text{BR}}^{(1)} \rangle \), and likewise, we obtain:

\[ \frac{\langle \hat{L}_x \rangle_{\text{PIA}}}{\langle \hat{L}_y \rangle_{\text{PIA}}} = \mp 2 \sqrt{2} \alpha_{\text{PIA}} \left( - \sin \varphi_q \cos \varphi_q \right). \] (19)

We note that the Rashba and PIA terms breaks parity symmetry, and as a consequence, the corrections in Eqs. (18) and (19) resemble the pseudomomentum and pseudodotorque defined in (6) and (7), respectively.

We now consider the axial correction due to \( \sigma \)-band mixing, \( \langle \hat{L}_\sigma \rangle_{\sigma} \). Eqs. (13), (14) and (15) yield three different second order contributions, which result into three terms proportional to \( \tau (\sigma_z) \), owing to the SL symmetry breaking,

\[ \langle \hat{L}_\sigma \rangle \simeq \left( (\alpha_{\text{BR}} + \alpha_{\text{PIA}})^2 - \alpha_{\text{AT}}^2 \right) \tau \sigma_z^0, \]

where the negative sign in front of the intrinsic SOC term indicates that spin ‘up’ (‘down’) electrons couple to (anti-)clockwise rotating \( p \)-orbitals within the \( \sigma \)-band, and the converse for the holes (see Fig. 1.b).

For completeness, we evaluate higher order corrections along the armchair direction, \( y \). Involved calculations yield third order corrections, (see Appendix F):

\[ \langle \hat{L}_y \rangle \simeq \alpha_{\text{AT}}^2 \alpha_{\text{BR}} \left( \hat{\sigma}_x \hat{s}_x + \tau \sigma_z^0 \hat{s}_y \right) + \alpha_{\text{AT}}^4 \tau (\hat{s}_y), \] (20)

In presence of inversion symmetry, \( \alpha_{\text{BR}} = \alpha_{\text{PIA}} = 0 \), the corrections along the armchair direction would only appear to third order, reflecting the intrinsic peculiarities of the lattice structure.

We have thus encountered striking anisotropies in the angular momentum corrections, which are first order along \( \hat{x} \), second order along \( \hat{z} \) and third order or higher along the armchair direction. Taking into account the correction of the \( \pi \) bands given in (11), we can summarize our result as:

\[ \langle \hat{L}_x \rangle \simeq \pm 2 \sqrt{2} \alpha_{\text{AT}} \tau \sigma_z^0 + (\alpha_{\text{PIA}} + \alpha_{\text{BR}}) s_z \tau \sin \varphi_q, \]
\[ \langle \hat{L}_y \rangle \simeq \mp 2 \sqrt{2} \alpha_{\text{PIA}} s_z \tau \cos \varphi_q, \]
\[ \langle \hat{L}_z \rangle \simeq \left[ \frac{\lambda_f}{\lambda_{\text{soc}}} - \alpha_{\text{AT}}^2 + (\alpha_{\text{BR}} + \alpha_{\text{PIA}})^2 \right] \tau \sigma_z^0 \] (21)

Although in an ideal, single-particle picture \( \langle \tau \sigma_z^0 \rangle = 0 \) and \( \langle \tau s_z^0 \rangle = 0 \) symmetry breaking terms would allow to resolve inherent internal structure of the Dirac carriers. For instance, electron-spin resonance on a graphene doped sample would allow to address directly the angular momentum correction. Since the value of the gap is known, \( 2 \lambda_f \simeq 42 \mu \text{eV} \), resolving \( g \)-tensor along the main crystallographic directions could be employed to find the value of atomic SOC, \( \lambda_{\text{soc}}^c \) or the magnitude of the Stark parameter, \( \lambda_z \).

III. CONCLUSIONS

We have considered a Dirac Hamiltonian in graphene with a mass term and we have obtained the finite angular momentum corrections along the main crystallographic axis. Intrinsic SOC causes the positive energy carriers (electrons) in one SL with spin ‘up’ to couple to anti-clockwise rotating orbitals, whereas those with spin ‘down’ couple to clockwise rotating orbitals, with the converse occurring for negative energy quasiparticles (holes). This confirms the CPT symmetry in the Hamiltonian, and, ultimately, reflects the chirality of the Dirac electrons. We have developed an intuitive connection between angular momentum and SL spin, where the axial quantization is given in terms of the sum of usual \( L_z \) operator and \( \nu \sigma_z \), with \( \nu \) being the winding number. This connection is very important when establishing the selection rules that dictate how Dirac carriers couple to other carrying angular momentum quasiparticles, such as photons. Corrections to the in-plane momentum are related to a pseudovector whose torque is perpendicular to the in-plane SL spin. In the absence of external SOC, we find first order corrections along the zig-zag direction, owing to the propagating \( p_d \) orbitals at DPs, whereas no corrections are observed in the armchair direction (up to third order). Whereas the intrinsic correction is associated with the pseudoscalar \( \tau \sigma_z \), the extrinsic correction is related to an in-plane pseudovector perpendicular to in-plane SL spin, \( \hat{\sigma}_\parallel \). The angular momentum correction anisotropy presented here has been confirmed in recent angle-resolved electron-spin resonance experiments [17].

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Appendix A: \( \hat{\sigma}_\parallel \) is not a pseudovector

A pseudovector or axial vector transforms like a polar vector under rotations, but gains a sign flip under improper rotations, such as parity inversion. Here, we show that \( \hat{\sigma}_\parallel \equiv (\tau \hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z) \) transforms as a polar vector, in spite of being expressed in terms of the Pauli matrices.
Under inversion symmetry, \( \mathcal{P} \), the sublattices \( A \) and \( B \) are switched, as well as the valleys, and hence, the Pauli matrices transform as \( \mathcal{P} : (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z) \rightarrow (\hat{\sigma}_x, -\hat{\sigma}_y, -\hat{\sigma}_z) \). Noting that the valleys are also switched, \( \mathcal{P} \mathcal{P} = -\mathcal{P} \), we obtain:

\[
\hat{\mathcal{P}} \hat{\sigma}_\tau = (-\tau \hat{\sigma}_x, -\tau \hat{\sigma}_y, -\tau \hat{\sigma}_z).
\]

We conclude that \( \hat{\sigma}_\tau \) is a polar vector, as well as the in-plane component, \( \hat{\sigma}_z \).

Hence, the first term of Eq. (1) is a scalar: it is straightforward to see that it is invariant under parity, as both \( \hat{q}_x \) and \( \hat{q}_y \) change sign under inversion transformation. The Semenov term, \( \varepsilon_{AB} \sigma_z \), is, however, a pseudoscalar, as opposed to the parity-preserving Kane-Mele term, \( \lambda_1 \hat{\tau} \hat{s}_z \).

It is tempting to express the Hamiltonian of Eq. (1) as a scalar product of \( \hat{\sigma}_\tau = (\tau \sigma_x, \sigma_y, \sigma_z) \) and \( \hat{q}_{3d} = (q_x, q_y, \lambda/\hbar v_F) \) by identifying \( q_z = \lambda/\hbar v_F \). However, \( \hat{q}_{3d} \) is neither a polar nor an axial vector, and the third component cannot be associated with a momentum, leading to unphysical interpretations.

**Appendix B: Constant of motion in Dirac Hamiltonians**

In the search for a generalization of Eq. (5) in other Dirac Hamiltonians, we focus on bilayer graphene. As MacCann et al. demonstrated, [37] quasiparticles in bilayer graphene can be described by using the effective Hamiltonian,

\[
\hat{H}_{BG} = -\frac{\hbar^2 q^2}{2m^*} \hat{\sigma}_\tau \hat{n}, \quad \hat{n} = (\cos 2\varphi_q, \sin 2\varphi_q)
\]

where the resulting eigenstates gain a phase shift of \( 2\pi \) under an adiabatic rotation of a closed contour in momentum space, corresponding to a Berry phase of \( 2\pi \) [38] (or a winding number \( \nu = 2 \)). The time evolution of \( \hat{\sigma}_z \) reads then:

\[
\frac{d\hat{\sigma}_z}{dt} = -i \frac{\tau \hbar q^2}{2m^*} \left\{ [\tau \hat{\sigma}_x \cos 2\varphi_q + \hat{\sigma}_y \sin 2\varphi_q, \hat{\sigma}_z] \right\} = \frac{\tau \hbar q^2}{m^*} (\tau \hat{\sigma}_y \cos 2\varphi_q - \hat{\sigma}_x \sin 2\varphi_q),
\]

and likewise, we have for \( \hat{L}_z \):

\[
\frac{d\hat{L}_z}{dt} = -i \frac{\tau \hbar^2 q^2}{2m^*} \left\{ [\tau \hat{\sigma}_x (\hat{q}_x^2 - \hat{q}_y^2) + 2\hat{\sigma}_y \hat{q}_x \hat{q}_y, \hat{x} \hat{q}_y - \hat{y} \hat{q}_x] \right\}

= \frac{\tau \hbar^2 q^2}{m^*} (\tau \hat{\sigma}_x \sin 2\varphi_q - \hat{\sigma}_y \cos 2\varphi_q) = -i \tau \hbar \hat{\sigma}_z,
\]

which is, combining (B1) and (B2),

\[
\frac{d}{dt}(L_z + i\tau \hbar \sigma_z) = 0,
\]

resulting in (5) for \( \nu = 2 \).

**Appendix C: The hybridized \( \pi \)-bands**

We consider the unperturbed eigenstates in terms of \( p_z \) orbitals (3). Using perturbation theory within the two-center Slater Koster approximation [39] we obtain the non-zero \( d \)-orbital contribution,

\[
|\varphi^{(1)}_d\rangle \simeq \frac{C_A}{\epsilon_{pd}} \left( V_{x_1}^{BA}(k) |d_{x_1}^A(k)\rangle + V_{y_1}^{BA}(k) |d_{y_1}^B(k)\rangle \right)

- \frac{C_B}{\epsilon_{pd}} \left( V_{x_2}^{AB}(k) |d_{x_2}^A(k)\rangle + V_{y_2}^{AB}(k) |d_{y_2}^B(k)\rangle \right).
\]

The matrix elements \( V_{ij}^{\alpha\beta}(k) \equiv \sum_a \langle d_{a,i}^\alpha | V^\beta | d_{a,j}^\beta \rangle \) are to be evaluated near the DPs, i.e., at \( \vec{k} = \vec{q} + \vec{K}^{(i)} \), with \( \vec{K} = -\vec{K}' = (4\pi/3\sqrt{3}a,0) \), and \( a \) being the distance between two NN \( 3 \)C atoms,

\[
(k_x, k_y) = \left( \frac{4\pi \tau}{3\sqrt{3}a} + q_x, q_y \right).
\]

The \( p - d \) hopping is described in terms of the NN directive cosines, \( \hat{d}_i = (\hat{l}_i, m_i) \) as depicted in Fig. 2. Those are \( \hat{d}_{1,2} = (\pm \sqrt{3}/2, -1/2) \) and \( \hat{d}_3 = (0,1) \), giving, e.g. for the coupling of \( d_{y_2}^B \) and \( p_z^A \) orbitals:

\[
V_{x_2,z}^{BA}(k) = V_{pd} \sum_i m_i e^{ik\hat{d}_i} = \frac{\sqrt{3}}{2} V_{pd} \left( e^{ik_{x_2}} - e^{ik_{y_2}} \right) e^{-i\frac{aq}{2}} = i \frac{3V_{pd}}{2} \sin \left( \frac{2\pi \tau}{3} + q_x a \sqrt{3} \right) \simeq i \frac{3V_{pd}}{2} \left( 1 - \frac{aq}{2} e^{i\pi q_x} \right),
\]

where we have used that \( V_{x_2,z} = iV_{pd}^z \). Likewise, we have:

\[
V_{y_1,x_2}^{BA}(k) = V_{pd} \sum_i m_i e^{ik\hat{d}_i} = \frac{1}{2} \left( e^{ik_{x_2}} - e^{-ik_{x_2}} \right) e^{-i\frac{aq}{2}} + e^{i\frac{aq}{2}} \simeq \frac{3V_{pd}}{2} \left( 1 + \frac{aq}{2} e^{i\pi q_x} \right).
\]
It is worth noting that under sublattice swap, the matrix elements change sign, that is, \( V_{iz,z}^{\alpha \beta}(k) = \sum_i V_{iz,z}^{\alpha \beta} e^{i(k \cdot l + k_y m_i)} = - \sum_i V_{iz,z}^{\beta \alpha} e^{-i(k \cdot l + k_y m_i)} \), since the directive cosines change sign (see Fig. 2):
\[
V_{iz,z}^{AB}(k) = - [V_{iz,z}^{AB}(k)]^* = - V_{iz,z}^{BA}(k).
\]
This has important consequences, implying that the topological character of the \( \pi \) bands is preserved. To lowest order, that is, neglecting the linear in momentum terms, we obtain:
\[
|\varphi_d^{(1)}(k)|^2 \approx - \frac{3V_{pdz}}{2\varepsilon_{pd}} \left[ c_A \left( d_{yz}^B + i\tau d_{zz}^B \right) + c_B \left( -d_{yz}^A + i\tau d_{zz}^A \right) \right] = - \frac{3i\tau V_{pdz}}{\sqrt{2}\varepsilon_{pd}} \left( c_A(2\tau)^B + c_B(2 - \tau)^A \right),
\]
where in the last step we have used the angular momentum representation, \( |l, m_l\rangle \), with \( l = 2 \) and
\[
|2 \pm 1\rangle = \frac{1}{\sqrt{2}} \left( |d_{zz}\rangle \pm i|d_{yz}\rangle \right).
\]

**Appendix D: The hybridized \( \sigma \) bands near DPs**

We consider the \( sp^2 \) hybridization via \( \sigma \) bonds near the DPs. The low-energy Hamiltonian can be evaluated within a reduced Hilbert space spanned by \( \{s^\alpha, p_x^\beta, p_y^\beta\} \), \( \alpha \neq \beta \), as dominant hopping within the \( \sigma \) band occurs between NN \( s \)- and \( p_{x,y} \)-orbitals [28]. The hopping between an \( s \)-orbital in SL A and \( p_x(p_y) \) in the SL B is given by \( l_i V_{sp\sigma}(m_i V_{sp\sigma}) \). Hence, we can employ the results of the previous section, where only the prefactor changes. Using Eq. (C1), we obtain:
\[
V_{s,sp}(k) \approx V_{sp\sigma} \sum_i l_i e^{i\vec{k}\vec{d}_i} = i\tau V_{sp\sigma} \left( 1 - \frac{aq}{2} e^{i\tau \varphi_A} \right)
\]
Likewise, we have:
\[
V_{s,p\gamma}(k) \approx \frac{3}{2} V_{sp\sigma} \left( 1 + \frac{aq}{2} \tau q_x + i q_y \right),
\]
and it follows, using symmetry arguments, \( V_{s,sp}(k) = -[V_{s,sp}(k)]^* \), that is:
\[
V_{s,sp}(k) \approx V_{s,p\gamma}(k) \approx \frac{3}{2} V_{sp\sigma} \left( 1 + \frac{aq}{2} \tau q_x - i q_y \right),
\]
In the basis spanned by \( \{s^A, |1, \tau\rangle^B, |1, -\tau\rangle^B\} \) with \( |1, \pm\tau\rangle^B = (|p_x^B\rangle \mp i\tau |p_y^B\rangle)/\sqrt{2} \), we have:
\[
\hat{H}_h^{BA} = \begin{pmatrix}
\varepsilon_s & 3i\tau V_{sp\sigma}/\sqrt{2} & 0 \\
-3i\tau V_{sp\sigma}/\sqrt{2} & \varepsilon_p & 0 \\
0 & 0 & \varepsilon_p
\end{pmatrix}, \tag{D1}
\]
with eigenvalues:
\[
\varepsilon_\sigma = \frac{\varepsilon_s + \varepsilon_p}{2} \pm \sqrt{\left( \frac{\varepsilon_s - \varepsilon_p}{2} \right)^2 + \frac{9V_{sp\sigma}^2}{4}}, \quad \varepsilon_0 = \varepsilon_p,
\]
and corresponding eigenvectors, with \( \phi^0_{AB} = |1 - \tau\rangle^B \) and
\[
\phi^{\pm}_{BA} = \begin{pmatrix} i\tau \cos \gamma \\ \sin \gamma \end{pmatrix}, \quad \phi^{-}_{BA} = \begin{pmatrix} -i\tau \sin \gamma \\ \cos \gamma \end{pmatrix}, \tag{D2}
\]
where we have defined
\[
\gamma = \arctan \left[ \frac{3V_{sp\sigma}}{\sqrt{2}(\varepsilon_s^+ - \varepsilon_p^+)} \right].
\]
Likewise, we have that in the basis spanned by \( \{s^B, |1, -\tau\rangle^A, |1, \tau\rangle^A\} \), the hopping Hamiltonian is formally identical to that of Eq. (D1), yielding same eigenvalues, and similar eigenvectors:
\[
\phi^+_{BA} = \begin{pmatrix} i\tau \cos \gamma \\ \sin \gamma \end{pmatrix}, \quad \phi^{-}_{BA} = \begin{pmatrix} -i\tau \sin \gamma \\ \cos \gamma \end{pmatrix}, \tag{D3}
\]
with \( \phi^0_{AB} = |1\tau\rangle^A \).

**Appendix E: PIA coupling**

We consider now the coupling induced by horizontal plane mirror asymmetry, PIA. The term arises in the presence of adsorbates, [33] ripples [32, 35] or other defects, and causes a coupling between the \( p_z \) and the NNs \( p_{x,y} \) orbitals [34]. We account for this term assuming a vertical relative component of one lattice with respect to the other, with a directive cosinus given by \( n_{AB} = n^B \cap i \). Employing the two-center Slater-Koster approximation [39], the relevant orbital matrix elements near DPs are \( V_{s,sp}(q) = \langle p^B_i|V_{p^A_j}\rangle \), with:
\[
V_{s,sp}(q) = \langle p^B_{p\sigma} - p_{p\sigma} \rangle \sum_i n_{i} l_i e^{i\vec{k}\vec{d}_i} = \frac{3n_{i} V_{sp\sigma}}{2} \left( 1 - \frac{aq}{2} e^{i\tau \varphi_A} \right),
\]
\[
V_{s,sp}(q) = \langle p^B_{p\sigma} - p_{p\sigma} \rangle \sum_i n_{i} l_i e^{i\vec{k}\vec{d}_i} = \frac{3n_{i} V_{sp\sigma}}{2} \left( 1 + \frac{aq}{2} e^{i\tau \varphi_A} \right),
\]
and
\[
V_{s,sp}(q) = \langle p^B_{p\sigma} - p_{p\sigma} \rangle \sum_i n_{i} l_i e^{i\vec{k}\vec{d}_i} = \frac{3n_{i} V_{sp\sigma}}{2} \left( 1 - \frac{aq}{2} e^{i\tau \varphi_A} \right),
\]
where we have employed the procedure of Eqs. (C1) and (C2), and \( n^B \) is a sublattice B vertical displacement. \( V_{n^B}(q) \) are trivially obtained, using \( V_{n^B}(q, n^A) = -(V_{n^A}(q, n^A))^\ast \). The allowed SOC term is then of the form \( \hat{L}_x \hat{s}_x + \hat{L}_y \hat{s}_y / 2 \), which results into the coupling of the \( p_z \)-orbitals to the \( \alpha \)-band is given by:

\[
\frac{1}{2} \langle 1 | \hat{A} \hat{V} | p_z^A \rangle \otimes (\hat{s}_x + i \tau \hat{s}_y) = \tau_l \delta_{s_x, \tau} \left( \frac{3n^B}{4} (V_{ppx} - V_{ppy}) \right),
\]

where the spin degree of freedom has been explicitly evaluated in terms of the valley, to ensure PT symmetry.

\[
\frac{1}{2} \langle 1 | \hat{A} \hat{V} | p_z^B \rangle \otimes (\hat{s}_x - i \tau \hat{s}_y) = \tau_l \delta_{s_x, \tau} \left( \frac{3n^A}{4} (V_{ppx} - V_{ppy}) \right),
\]

Appendix F: Third order corrections

We consider the \( \hat{H}^{BR} + \hat{H}^{soc} \) and calculate the corrections over \( |\phi^{(1)}_{soc}\rangle \) and \( |\phi^{(1)}_{BR}\rangle \), which are the second order corrections to the WF:

\[
|\phi^{(2)}\rangle \simeq \alpha_{soc}^2 \left[ c_A \langle \tau \hat{s}_x + i \tau \hat{s}_y \rangle |p_z^A\rangle - c_B \langle -\tau \hat{s}_x + i \tau \hat{s}_y \rangle |p_z^B\rangle \right]
- i \alpha_{BR} \alpha_{soc} \left[ c_A \langle -\tau \hat{s}_x + i \tau \hat{s}_y \rangle |p_z^B\rangle + c_B \langle \tau \hat{s}_x + i \tau \hat{s}_y \rangle |p_z^A\rangle \right],
\]

where \( \langle \rangle^n \) indicates that the expectation value is to be calculated in SL \( \alpha \). The next order correction to angular momentum along \( y \) would be \( 2R \left\{ (\phi^{(1)}_{\sigma} | \hat{L}_y | \phi^{(2)}_{\sigma}) \right\} \), yielding:

\[
\langle \hat{L}_y \rangle \simeq \alpha_{soc}^3 \tau (\hat{s}_y^A | c_A |^2 + \hat{s}_y^B | c_B |^2) +
\alpha_{soc}^2 \alpha_{BR} \left( \tau \epsilon_{A} c_{B} \hat{s}_x^A + \tau c_{A} \epsilon_{B} \hat{s}_x^B +
+ i \alpha_{A} \epsilon_{B} \hat{s}_y^A - i \alpha_{A} \epsilon_{B} \hat{s}_y^B \right).
\]

In absence of spin-SL coupling, we can consider \( \langle \hat{s}_i \rangle^A = \langle \hat{s}_i \rangle^B = \langle \hat{s}_i \rangle, i = x, y \). Using that \( |c_A|^2 + |c_B|^2 \simeq 1 \) and (3), we obtain (20).

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