**sp-band tight-binding model for the Bychkov-Rashba effect in a two-dimensional electron system including nearest-neighbor contributions from an electric field**

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We present a tight-binding calculation for a two-dimensional electron gas (2DEG) including the spin-orbit interaction as well as an electric field perpendicular to the system in order to model the Bychkov-Rashba spin splitting. The associated potential gradient introduces two contributions to the tight-binding matrix: an on-site contribution coupling orbitals of the same atom and a nearest-neighbor contribution. At the $T$ point the first-order Rashba constant $\alpha_R$ only depends on this nearest-neighbor contribution regardless of the lattices considered (square, hexagonal, honeycomb). Applying the model to graphene reveals that this nearest-neighbor contribution induces a significant increase in the zeroth-order Rashba constant $\lambda_R$ and introduces a spin-splitting component, which varies linearly in momentum.

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I. INTRODUCTION

The Bychkov-Rashba (BR) model has been remarkably successful in qualitatively describing the lifting of the spin degeneracy in a two-dimensional (2D) electron gas by means of a perpendicular electric field. However, it is a phenomenological model that does not include the atomic spin-orbit interaction or any details about the potential landscape of the crystal lattice. Therefore the electric field that enters the first-order Rashba constant $\alpha_R$ has to be regarded as an effective field whose magnitude cannot be predicted based on the BR model. Petersen and Hedegård have related the first-order Rashba coupling constant $\alpha_R$ to the parameters of a simple $p$-band tight-binding model including spin-orbit coupling which enabled them to make quantitative predictions for the size of the spin splitting.

In their model, the atomic spin-orbit coupling enters through the L $\cdot$ S Hamiltonian and the potential gradient results in a nonzero overlap of the in-plane $p_x$ and $p_y$ orbitals with the out-of-plane $p_z$ orbital of a neighboring atom. The first-order Rashba constant $\alpha_R$ then depends on the atomic spin-orbit coupling parameter $\alpha$ as well as a parameter $\gamma$ accounting for the influence of the potential gradient perpendicular to the 2D system. This potential gradient may also be interpreted in terms of an effective field resulting from an asymmetric hybridization of orbitals at the surface.

Recently, the tight-binding approach has also been used to describe the Rashba-type spin splitting in graphene. Here as well, the effective spin-orbit coupling parameter $\Delta So$ as well as the zeroth-order Rashba parameter $\lambda_R$ accounting for an electric field perpendicular to the graphene plane have been expressed analytically in terms of the tight-binding parameters. Konschuh et al. also considered contributions from $d$ orbitals, but they did not directly consider the nearest-neighbor contribution from the electric field. For graphene, so far, the nearest-neighbor contribution of the electric field has only been considered phenomenologically. This phenomenological model has already been successfully applied to honeycomb lattices as well as the Au(111) surface. A contribution from the electric field is expected from a coupling of orbitals in neighboring atoms as already indicated by Petersen and Hedegård yielding the same effective Hamiltonian as the phenomenological model. The question arises how the different on-site and nearest-neighbor contributions can be unified on common grounds.

Here, we present a generalization of the $sp$-band tight-binding models used for graphene as well as the one presented by Petersen and Hedegård. We calculate the effect of a constant potential gradient $\xi$ in the direction perpendicular to the 2D electron system ($z$ direction) separated into a contribution from the orbitals within the same atom as well as a contribution from orbitals of neighboring atoms. While the on-site contribution couples orbitals according to the well-known dipole selection rules $\Delta l = \pm 1$ and $\Delta m = 0$, the contribution from neighboring atoms also couples orbitals with $\Delta l = 0$ and $\Delta m \neq 0$. We will discuss the findings for the model system graphene, where additional interesting contributions to the Rashba parameter emerge. Finally, we apply this model to the band structure at the $T$ point in different two-dimensional lattices.

II. TIGHT-BINDING MODEL

The Hamiltonian that we employ can be divided into three different contributions:

$$H = H^b + H^{SOC} + H^\xi. \quad (1)$$

The first term is the tight-binding Hamiltonian describing the band structure in the linear combination of atomic orbitals (LCAO) approximation. Here, we will only consider $s$ and $p$ orbitals with on-site contributions $\epsilon_s$ and $\epsilon_p$, respectively. The tight-binding parameters describing the orbital overlap from neighboring atoms are $V_{ss}, V_{sp}, V_{pp}$, and $V_{pp}. The corresponding matrix is then

$$H^b_{o,o'} = \epsilon_o \delta_{o,o'} + \sum_{(i)} e^{AR}_i E(o,o',R_i). \quad (2)$$

Here, $o$ and $o'$ are the orbitals ($s$, $p_x$, $p_y$, $p_z$) in the tight-binding matrix and $\delta_{o,o'}$ is the Kronecker $\delta$. In the second term of Eq. (2), $E(o,o',R_i) = \langle o|H^b|o',R_i\rangle$ is an element from Table I. $(i)$ denotes the sum over neighboring atoms with $R_i$ being the vector connecting two neighboring atoms. If there

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TABLE I. Matrix elements for the $s$ and $p$ orbitals (Ref. 10). Values that are not given can be obtained by cyclic permutation. The quantities $u$, $v$, and $w$, which depend on the vector $\mathbf{R}$, connecting two neighboring atoms, are the directional cosines in the $x$, $y$, and $z$ direction, respectively. It should be noted that matrix elements with same (different) parity between orbitals transform even (odd) under exchange of indices [$(E(o',o, -\mathbf{R}) = (-1)^{l-l'}E(o,o', \mathbf{R})$].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Overlap</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E(s,s,\mathbf{R})$</td>
<td>$V_{ss}$</td>
</tr>
<tr>
<td>$E(s,p_{\alpha},\mathbf{R})$</td>
<td>$uV_{sp}$</td>
</tr>
<tr>
<td>$E(p_{\alpha},p_{\beta},\mathbf{R})$</td>
<td>$u^2V_{pp} + (1 - u^2)V_{pp'}$</td>
</tr>
<tr>
<td>$E(p_{\alpha},p_{\beta},\mathbf{R})$</td>
<td>$uv(V_{pp'} - V_{pp})$</td>
</tr>
</tbody>
</table>

is more than one atom in the basis, the matrices have to be adapted accordingly.

The term $H_{SOC}$ in Eq. (1) is the atomic spin-orbit interaction (see, e.g., Ref. 2),

$$
H_{SOC} = \alpha \mathbf{L} \cdot \mathbf{S} = \alpha \left[ \begin{array}{cccc}
0 & -i & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & -i & 0 \\
i & 0 & 0 & 0
\end{array} \right].
$$

Here the basis of the matrix is \{p_{\uparrow}, p_{\downarrow}, p_{\uparrow}, p_{\downarrow} \}.

The third contribution $H^z$ in Eq. (1) takes into account the potential gradient $\xi$ in the $z$ direction perpendicular to the 2D electronic structure, which resides in the $xy$ plane:

$$
H^z = \xi z.
$$

In order to adapt the Hamiltonian $H^z$ to the tight-binding framework, we divide the contributions from the Hamiltonian $H^z$ into an on-site part $H_{soc}^{\text{ onsite}}$ as well as a part coming from neighboring atoms $H_{soc}^{\text{neigh}}$.

In order to calculate the full integral, we use spherical harmonics for the angular part of the wave function. The radial part is approximated by the asymptotic radial wave function $R_0$ as outlined by Slater in Ref. 11:

$$
R_0(n^*, Z - s, r) \propto R_0 \left( \frac{r}{d_0} \right)^{n^* - 1} e^{-[(Z-s)/n^*]^{1/3}}.
$$

Here $n^*$ is an effective principal quantum number, $Z$ is the atomic number, $s$ is a screening charge, and $d_0 = 0.529 \text{ Å}$ is the Bohr radius (for details see Ref. 11). Further, we introduce a sign parameter $p_{nl} = (-1)^{n-l-1}$ to ensure an asymptotic approach to zero from positive or negative values. Here, $n$ and $l$ are the principal and orbital quantum numbers, respectively. This asymptotic wave function $R_0$ gives a reasonable approximation for the general behavior of the different tight-binding parameters that will be discussed in the following.

III. ON-SITE CONTRIBUTION FROM $H^z$

The matrix elements for the on-site Hamiltonian $H_{soc}^{\text{ onsite}}$ can be written as

$$
H_{soc}^{\text{ onsite}} = \langle o | \xi z | o' \rangle = \xi \langle o | r \cos \theta | o' \rangle.
$$

Here, $r$ is the radial component in spherical coordinates and $z = r \cos \theta = 2 \sqrt{\pi} r Y_1^0(\theta, \phi)$ represents the conversion from Cartesian to spherical coordinates and to spherical harmonics, respectively. The last step allows us to express the angular part of the integral in Eq. (5) in terms of Gaunt coefficients. From the properties of the Gaunt coefficients, we can directly deduce that the matrix elements in $H^z$ are only nonzero, if $\Delta l = \pm 1$ and $\Delta m = 0$. Furthermore, as the orbitals with $m \neq 0$ are a linear combination of the spherical harmonics, some matrix elements even cancel to zero for $\Delta m = 0$. According to these selection rules the only nonzero elements are $sp_z, p_d z, p_j d_z$, and $p_l d_z$.

In order to account for the effects of the potential gradient on the on-site contribution, we define a parameter $\gamma_{sp}$ in analogy to Ref. 2. Using Eq. (4), we find

$$
\gamma_{sp} = \langle s | z | p_z \rangle = -a_0 n^* (1 + 2 n^*)
\frac{2 \sqrt{5} (Z - s)}{n^*}.
$$

It serves as an empirical parameter similar to the tight-binding parameters, e.g., $V_{sp}$. The parameter $\gamma_{sp}$ depends on the effective principal quantum number $n^*$ through the radial part of the wave function, which defines the spatial extent of the orbital. The parameter $\gamma_{sp}$ is shown in Fig. 1 as a function of the principal quantum number $n$. The modulus for $\gamma_{sp}$ continuously increases with the effective principal quantum number $n^*$, i.e., the parameter becomes more important for heavier atoms. The increase with $n^*$ can be understood by the increasing spatial extension of the wave function, so that it becomes more sensitive to the effects of the potential gradient. The modulus of $\gamma_{sp}$ is closely related to the position of the principal maximum $r_{max} = a_0 n^*/(Z - s)$ of the radial charge density $\rho_r \propto r^2 R_n$.
IV. NEAREST-NEIGHBOR CONTRIBUTION FROM $H^z$

The matrix elements for the $H_{\text{z,neigh}}$ Hamiltonian between two neighboring atoms are

$$H_{\text{z,neigh}} = \sum_{\langle i \rangle} e^{i \mathbf{k} \mathbf{R}_i} \xi \langle \alpha | \xi | \alpha' , \mathbf{R}_i \rangle = \sum_{\langle i \rangle} e^{i \mathbf{k} \mathbf{R}_i} \xi \langle \alpha | r \cos \theta | \alpha' , \mathbf{R}_i \rangle. \quad (7)$$

These integrals can only be evaluated numerically even for the rather simple wave function of the hydrogen atom. Nevertheless, we can identify the nonzero matrix elements in $H_{\text{z,neigh}}$ and find their angular dependence in terms of the directional cosines. The resulting tight-binding matrix for the contribution of the neighboring atoms to the potential gradient in the basis $\{s, p_x, p_y, p_z\}$ is

$$H_{\text{z,neigh}} = \sum_{\langle i \rangle} e^{i \mathbf{k} \mathbf{R}_i} \xi \begin{pmatrix} 0 & u\varphi_{s,p} \gamma_{s,p} & v\varphi_{s,p} \gamma_{s,p} & (1 - w^2)\varphi_{s,p} \gamma_{s,p} + w^2\varphi_{s,p} \\ 0 & 0 & 0 & u\varphi_{p,p} \gamma_{p,p} \\ (1 - w^2)\varphi_{s,p} \gamma_{s,p} + w^2\varphi_{s,p} & -u\varphi_{p,p} \gamma_{p,p} & -v\varphi_{p,p} \gamma_{p,p} & 0 \\ -u\varphi_{p,p} \gamma_{p,p} & -v\varphi_{p,p} \gamma_{p,p} & 0 & 0 \end{pmatrix}. \quad (8)$$

The quantities $u$, $v$, and $w$, which depend on the vector $\mathbf{R}_i$ connecting two neighboring atoms, are the directional cosines in the $x$, $y$, and $z$ direction, respectively. The parameters $\gamma_{s,p}$, $\gamma_{p,s}$, and $\gamma_{p,p}$ are defined as

$$\gamma_{s,p} = \langle s | z | p_z, d\mathbf{e}_z \rangle,$$

$$\gamma_{p,s} = \langle p_z, d\mathbf{e}_z | z | s \rangle,$$

$$\gamma_{p,p} = \langle p_z, d\mathbf{e}_z | p_z, d\mathbf{e}_z \rangle,$$ \quad (9)

where $d$ is the nearest-neighbor distance and $\mathbf{e}_z$ are the unit vectors in the respective directions. A matrix element in $H_{\text{z,neigh}}$ will transform even (odd) under exchange of indices if the orbitals have different (same) parity, i.e., $E_r(\alpha', \alpha, -\mathbf{R}_i) = (-1)^{|\ell - l'|} E_r(\alpha, \alpha', \mathbf{R}_i)$. The parameter $\gamma_{s,p}$ accounts for the nearest-neighbor displacement perpendicular to the $xy$ plane. To calculate $\gamma_{s,p}$, the $xy$ plane ($z = 0$) has been set at an equal distance between the neighboring atoms for the influence of the potential on the two neighboring atoms to be equal. Equation (8) applies to the general case of a corrugated 2D system where the vectors connecting the atoms have a $z$ component. If the 2D system is completely flat, then $w \to 0$ and the matrix in Eq. (8) reduces to

$$H_{\text{z,neigh}} = \sum_{\langle i \rangle} e^{i \mathbf{k} \mathbf{R}_i} \xi \begin{pmatrix} 0 & \varphi_{s,p} \gamma_{s,p} & \varphi_{p,p} \gamma_{p,p} & (1 - w^2)\varphi_{s,p} \gamma_{s,p} + w^2\varphi_{s,p} \\ 0 & 0 & 0 & \varphi_{p,p} \gamma_{p,p} \\ \varphi_{s,p} \gamma_{s,p} & -\varphi_{p,p} \gamma_{p,p} & 0 & 0 \\ -\varphi_{p,p} \gamma_{p,p} & 0 & 0 & 0 \end{pmatrix}. \quad (10)$$

The matrix in Eq. (10) depends on the parameters $\gamma_{s,p}$ and $\gamma_{p,p}$, which account for a lattice residing in the $xy$ plane. If we further reduce the basis to the $p$ orbitals in the lower matrix of Eq. (7), we recover the parameter $\gamma$ from the potential gradient that was used by Petersen and Hedegård, i.e., $\gamma = \xi \varphi_{p,p}$. In contrast to the on-site contribution of the potential gradient, where only orbitals with $\Delta l = \pm 1$ couple, the contribution from the neighboring atoms also couples orbitals with $\Delta l = 0$ and $\Delta m \neq 0$.

The parameters $\gamma_{p,p}$, $\gamma_{p,s}$, and $\gamma_{p,p}$ all depend on the distance dependence between the neighboring atoms. In order to plot this distance dependence (Fig. 2) we use the asymptotic radial wave function $R_a$ for the carbon atom. The parameters $\gamma_{p,p}$ and $\gamma_{p,p}$ have a maximum at zero distance, which is expected as they are closely related to the only nonzero on-site contribution $\gamma_{p,p}$. The third parameter $\gamma_{p,p}$ reaches a maximum for a certain distance $d$ between neighboring atoms indicating optimal overlap. For larger distances all three parameters decrease to zero as the overlap between orbitals diminishes.

V. APPLICATION TO GRAPHENE AT $K$

We apply this model to the honeycomb lattice of graphene. A Rashba-type spin splitting has been discussed extensively in the literature, but the combined aspects of an on-site as well as a nearest-neighbor contribution to the potential gradient have not been considered so far.

The basis vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ as well as the vector $\tau$ connecting the two basis atoms ($A$ and $B$) can be defined using the nearest-neighbor distance $d$:

$$\mathbf{a}_1 = \frac{d}{2} \left( -\sqrt{3} \begin{array}{c} \sqrt{3} \\ 3 \end{array} \right) , \quad \mathbf{a}_2 = \frac{d}{2} \left( \sqrt{3} \begin{array}{c} 0 \\ 1 \end{array} \right) , \quad \tau = d \begin{array}{c} 0 \\ 1 \end{array} . \quad (11)$$

With $s$ and $p$ orbitals, two basis atoms, and two spin components, the resulting matrix will be a $16 \times 16$ matrix. In

FIG. 2. (Color online) Dependence of the parameters $\gamma_{p,p}$, $\gamma_{p,s}$, and $\gamma_{p,p}$ on the distance $d$ between the neighboring atoms. The calculations have been done for the valence orbitals of carbon.
order to compare the results from the Hamiltonian in Eq. (1) to previous results, we project, i.e., downfold, the Hamiltonian in Eq. (1) onto the \( p_z \) bands near the \( \overline{K} \) point using a standard theorem:

\[
H^\text{eff} = P H P + \frac{P H Q}{\varepsilon - Q H Q} Q H P. \tag{12}
\]

Here, \( P \) is a matrix projecting the Hamiltonian near the energy \( \varepsilon \) onto the \( p_z \) orbitals and \( Q = 1 - P \). The denominator in the second term of Eq. (12) will be evaluated at the \( \overline{K} \) point with \( \alpha = 0 \) and \( \xi = 0 \). The elements of the resulting \( 4 \times 4 \) matrix

\[
H^\text{eff} = \begin{pmatrix}
H_{11} & H_{12} & H_{13} & H_{14} \\
H_{12}^* & H_{22} & H_{23} & H_{24} \\
H_{13}^* & H_{23}^* & H_{33} & H_{34} \\
H_{14}^* & H_{24}^* & H_{34}^* & H_{44}
\end{pmatrix}, \tag{13}
\]

with the basis \( \{p_{z1A}, p_{z1B}, p_{z2A}, p_{z2B}\} \), are to second order in momentum \( k \):

\[
\begin{align*}
H_{11} &= -d^2(k_x^2 + k_y^2)\xi^2 \gamma_{\text{pp1}}(V_{\text{sp}}\gamma_p + \gamma_{\text{pp1}}\varepsilon_s)/2V_{\text{sp}}^2 + \xi^2 \gamma_{\text{pp1}}(2V_{\text{sp}}\gamma_p + \gamma_{\text{pp1}}\varepsilon_s)/V_{\text{sp}}^2, \\
H_{12} &= \frac{3}{2}d(k_x - ik_y)\left(V_{\text{ppp}} + \xi^2 \gamma_{\text{pp1}}V_{\text{sp}}/V_{\text{sp}}^2\right) + \frac{3}{8}d^2(k_x + ik_y)^2\left[V_{\text{ppp}} - 2\xi^2 \gamma_{\text{pp1}}\left(V_{\text{ppp}} - \gamma_{\text{pp1}}/V_{\text{sp}}\right)\right], \\
H_{13} &= -id^2(k_x + ik_y)\frac{\alpha\xi}{8} \left(V_{\text{ppp}} - \gamma_{\text{pp1}}/V_{\text{sp}}\right) + d(ik_x + k_y)\frac{\alpha\xi}{2} \left(V_{\text{ppp}} - \gamma_{\text{pp1}}/V_{\text{sp}}\right), \\
H_{14} &= 0, \\
H_{22} &= -d^2(k_x^2 + k_y^2)\xi^2 \gamma_{\text{pp1}}(V_{\text{sp}}\gamma_p + \gamma_{\text{pp1}}\varepsilon_s)/2V_{\text{sp}}^2 + 18V_{\text{sp}}\xi^2 \gamma_{\text{pp1}}\gamma_p + (\alpha^2 + 9\xi^2\gamma_{\text{pp1}}^2)\varepsilon_s/9V_{\text{sp}}^2, \\
H_{23} &= id^2(k_x^2 + k_y^2)\frac{\alpha\xi \gamma_{\text{pp1}}\varepsilon_s}{6V_{\text{sp}}^2} - 2d\frac{\alpha\xi (V_{\text{sp}}\gamma_p + \gamma_{\text{pp1}}\varepsilon_s)}{3V_{\text{sp}}^2}. \tag{14}
\end{align*}
\]

In order to better understand the origin of the different terms in Eq. (14) and their effect on the band dispersion, we compare the matrix elements in Eq. (14) to the Hamiltonian expressed in terms of the basis functions of the trigonal graphene band structure near the \( \overline{K} \) point from Ref. 14:

\[
H^\text{sym} = a_{10} + a_{61}(k_x s_x + k_y s_y) + a_{11}(k_x^2 + k_y^2) + a_{62}\left[(k_y^2 - k_x^2)s_x + 2k_x k_y s_y\right] + \alpha p_{21} s_x s_z + \alpha p_{22}(k_x^2 + k_y^2)s_x s_z + \xi r_{23}(k_y^2 - k_x^2)\gamma_{\text{sp}} + (k_x^2 + k_y^2)s_x s_y + \xi r_{63}(k_x^2 + k_y^2)s_x s_y + \xi r_{65}(k_x^2 + k_y^2)s_x s_y, \tag{15}
\]

For brevity, the superscripts of the coefficients in Ref. 14 as well as the unit matrices have been omitted. The \( s_i \) and \( \sigma_i \) (\( i = x, y, z \)) are the Pauli spin and pseudospin matrices, respectively. The coefficients \( a_{ij}, p_{ij}, \) and \( r_{ij} \) refer to the intrinsic band dispersion, the spin-orbit coupling \( \alpha \), and the effects of an external electric field \( \xi \) along the \( z \) direction, respectively. We find a direct correspondence between the Hamiltonian \( H^\text{eff} \) and \( H^\text{sym} \):

\[
\begin{align*}
a_{10} &= \frac{2\xi^2 \gamma_{\text{pp1}}\gamma_p}{V_{\text{sp}}^2} + \frac{(\alpha^2 + 18\xi^2 \gamma_{\text{pp1}}^2)\varepsilon_s}{18V_{\text{sp}}^2}, \\
a_{11} &= -(\alpha^2 + 18\xi^2 \gamma_{\text{pp1}}^2)\varepsilon_s/18V_{\text{sp}}^2, \\
a_{61} &= 3dV_{\text{ppp}} + 2\xi^2 \gamma_{\text{pp1}}V_{\text{ppp}}/V_{\text{sp}}^2, \\
a_{62} &= -\frac{3}{8}d^2\left[V_{\text{ppp}} - 2\xi^2 \gamma_{\text{pp1}}V_{\text{ppp}}/V_{\text{sp}}^2\right]V_{\text{sp}}^2, \\
p_{21} &= -\frac{\alpha\xi}{18V_{\text{sp}}^2}, \\
p_{22} &= 0, \\
r_{11} &= -\frac{d\alpha}{2}\left(V_{\text{ppp}} - \gamma_{\text{pp1}}/V_{\text{sp}}\right), \\
r_{12} &= -i\frac{d^2\alpha}{8}\left(V_{\text{ppp}} - \gamma_{\text{pp1}}/V_{\text{sp}}\right), \\
r_{62} &= \frac{\alpha\xi}{3V_{\text{sp}}^2} + \frac{\gamma_{\text{pp1}}\varepsilon_s}{3V_{\text{sp}}^2}, \\
r_{64} &= 0, \\
r_{65} &= 0, \\
p_{22} &= -\frac{d^2\alpha}{12}\frac{\gamma_{\text{pp1}}\varepsilon_s}{V_{\text{sp}}^2}. \tag{16}
\end{align*}
\]

All terms in Eq. (16) are influenced by the electric field \( \xi \) (through the parameters \( \gamma_{\text{pp1}} \) and/or the atomic spin-orbit coupling strength \( \alpha \) to second order, i.e., \( \alpha^2, \alpha \xi, \) or \( \xi^2 \)). The coefficients for the unperturbed band dispersion \( a_{ij} \) are corrected by terms proportional to \( \xi^2 \) and/or \( \alpha^2 \) from the nearest-neighbor contributions to the Hamiltonian \( H^2 \). Terms to second order in \( \xi \) and \( \alpha \) have not explicitly been considered in the expansion of the basis functions in Ref. 14. They result
from the projection of the Hamiltonian [Eq. (1)] and are thus
included for completeness. This affects the value of the band
velocity $h v_F$ related to $a_{61}$ as well as second-order corrections
to the linear band dispersion from the coefficients $a_{11}$ and
$a_{62}$. The coefficient $a_{10}$ is a constant offset corresponding to
a rigid-band shift, which has no further consequence for the
subsequent discussion. For the coefficients associated with
the spin-orbit interaction $p_{ij}$, the present tight-binding model
contributes only to second order in the atomic spin-orbit
coupling strength $\alpha$ via the parameter $p_{21}$. This result has
been obtained previously.\(^5\)

The coefficients $r_{ij}$ are related to the first-order contribution
of the electric field $\xi$. They also depend linearly on the
spin-orbit coupling $\alpha$. The coefficient $r_{62}$ can be identified
with the zeroth-order Rashba constant $\lambda_R$ (see, e.g., Refs. 4
and 5). Aside from the first term in $r_{62}$, which originates
from the on-site contribution in $H^z$, all other contributions to
$r_{ij}$ come from the nearest-neighbor contribution. The on-site
contribution in $r_{62}$ has been considered in previous models\(^4,5\)
and can be constructed from the effective on-site Rashba term:\(^6\)

$$H^{\text{on-site}} = V_R (s_z \sigma_z - s_x \sigma_x), \quad (17)$$

where $V_R$ is the corresponding effective coupling constant,
with $V_R = a_2 \xi \gamma_{sp}$. The second term in $r_{62}$ has not been
considered in previous models.\(^5\) It is of the same order of
magnitude as the first (on-site) term, but originates from the
nearest-neighbor contribution in $H^z$. It can be constructed from
the effective nearest-neighbor Rashba term to zeroth order in
momentum $k$, which has been discussed in Ref. 6 and in more
detail in Ref. 14:

$$H^{\text{neigh}} = \begin{pmatrix} 0 & h_R \\ h_R^* & 0 \end{pmatrix}, \quad h_R = V_R \sum_{(ij)} e^{i R_{ij}} (s \times \frac{R_i}{|R_i|}) \cdot \hat{z}, \quad (18)$$

where the sum is over nearest neighbors, $V_R$ is the corre-
sponding effective coupling constant, $\hat{z}$ is the unit vector
in the $z$ direction, and $s$ is the vector of Pauli matrices.\(^6,14\)
The second term in $r_{62}$ opens up a new path in the effective
nearest-neighbor hopping of two $p_z$ orbitals in addition to
the one discussed in Ref. 4. This means that the effect of the
electric field $\xi$ on the spin-splitting in graphene is larger than
previously assumed. Further, the effective nearest-
neighbor Rashba term in Eq. (18) has nonzero coefficients,
which are zero in the tight-binding model ($r_{63}$ and $r_{64}$). The
coefficients extracted from Eq. (18) are up to second order in
momentum $k$:

$$\begin{align*}
\xi r_{62} &= \frac{3}{2} V_R', \\
\xi r_{63} &= \frac{3}{2} d V_R', \\
\xi r_{64} &= \frac{3}{8} d^2 V_R'.
\end{align*} \quad (19)$$

Here, $V_R' = a_2 \xi \gamma_{sp} \gamma_{\text{p}} / 6 \gamma_{\text{p}}$. When comparing the coefficients to the
tight-binding model. Other contributions not considered in
the present tight-binding model (e.g., higher-order orbitals)
may result in nonzero coefficients $r_{63}$ and $r_{64}$. On the other
hand, the coefficient $r_{11}$ is nonzero in the tight-binding model,
but cannot be constructed from either Eqs. (17) or (18).\(^4,14\)

It can be assigned to the “linear” Rashba constant $a_R$ from
the “conventional” Bychkov-Rashba model,\(^3\) as the corre-
sponding basis function shows the same linear momentum
dependence. It introduces a spin-dependent correction to the
band velocity $h v_F$. The coefficients $r_{12}$ and $r_{65}$ both give
a correction to second order in momentum. In this way,
the tight-binding model unifies different phenomenological
descriptions [Eqs. (17) and (18)] demonstrating that even
though they have similar effects on the band dispersion,
they actually have a different origin (the on-site and nearest-
neighbor contribution, respectively).

In order to make the effects of the different contributions
more obvious we reduce the Hamiltonian $H'^{\text{eff}}$ in Eqs. (13)
and (14) to first order in momentum $k$. This enables us to
calculate the energy eigenvalues in an analytical form. We find

$$\begin{align*}
E_{\mu, \lambda}(k) &= a_{61} + \lambda \xi r_{62} + \mu \sqrt{k^2 (a_{61} + \lambda \xi r_{11})^2 + (p_{21} - \lambda \xi r_{62})^2}, \quad (20)
\end{align*}$$

where $\mu = \pm 1$ refers to the valence/conduction band
and $\lambda = \pm 1$ is the index for the spin eigenstate. The origin
of the momentum $k$ is set at the $\overline{K}$ point. We can associate the coefficients of the basis functions with the band velocity $h v_F$,
the intrinsic spin-orbit splitting $\Delta_{\text{SOC}}$, as well as the zeroth
and first-order Rashba constants $\lambda_R$ and $a_R$:

$$\begin{align*}
\xi r_{62} &= a_{61} + \lambda \xi r_{62} = \frac{3}{2} d \left( V_{\text{ppp}} + \frac{\gamma_{\text{p}}}{\gamma_{\text{sp}}} \frac{\gamma_{\text{sp}}}{V_{\text{sp}}} \right), \\
\xi r_{11} &= \lambda \xi r_{11} = \frac{\alpha \xi}{2} \left( \frac{\gamma_{\text{pp}}}{V_{\text{pp}} - V_{\text{sp}}} - \frac{\gamma_{\text{sp}}}{V_{\text{sp}}} \right),
\end{align*} \quad (21)$$

For a numerical evaluation of the parameters in Eq. (21), we
have to calculate the potential gradient parameters $\gamma_{\text{pp}}$, $\gamma_{\text{sp}}$, and $\gamma_{\text{ppp}}$ using Eqs. (6) and (9). Again, we use the asymptotic
radial wave function $R_0$ for the carbon atom. Further, for the
atomic spin-orbit coupling strength we assume $\alpha = 8.5$ meV,\(^5\)
and for the electric field we estimate $\xi = 0.1 \frac{e V}{\text{Å}}$, which is a reasonable value for a graphene layer on a substrate.
With the potential gradient parameters $\gamma_{\text{pp}} = -0.47 \text{ Å}$, $\gamma_{\text{sp}} = -0.16 \text{ Å}$, and $\gamma_{\text{ppp}} = 0.17 \text{ Å}$, as well as the tight-binding
parameters from Table II, we find at the $\overline{K}$ point

$$\begin{align*}
h v_F &= -6.46 \text{ eV} + \lambda \times 107.7 \text{ µeV Å}, \\
\Delta_{\text{SOC}} &= 1.14 \text{ µeV}, \\
\lambda_R &= 37.4 \text{ µeV}, \\
a_R &= 6.46 \text{ µeV Å}.
\end{align*} \quad (22)$$
TABLE II. Tight-binding parameters of graphene with a nearest-neighbor distance of $d = 1.42$ Å (Refs. 5 and 16).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\epsilon_s$</td>
<td>-8.868</td>
</tr>
<tr>
<td>$\epsilon_p$</td>
<td>0.000</td>
</tr>
<tr>
<td>$V_{ss0}$</td>
<td>-6.769</td>
</tr>
<tr>
<td>$V_{sp0}$</td>
<td>5.580</td>
</tr>
<tr>
<td>$V_{pp0}$</td>
<td>5.037</td>
</tr>
<tr>
<td>$V_{pp1}$</td>
<td>-3.033</td>
</tr>
</tbody>
</table>

The band velocity $\hbar v_F$ agrees with experimental values (see, e.g., Ref. 17). The band dispersion near the $\Gamma$ point is shown in Fig. 3 for different scenarios. It is clearly visible that the nearest-neighbor parameters $\gamma_{sp1}$ and $\gamma_{pp1}$ give a sizable contribution to the spin splitting. Away from the $\Gamma$ point, we find for the momentum dependent energy splitting $\Delta E$ between the spin-split branches

$$\Delta E = 2\lambda_R + 2|k|\alpha_R.$$  \hfill (23)

Therefore the nearest-neighbor contribution to the Hamiltonian $H^2$ does not only give a correction to the constant spin splitting, but also introduces an additional term, which depends linearly on momentum.

VI. APPLICATION TO $p_z$ BANDS AT $\Gamma$

We have carried out a similar analysis for the $p_z$ bands at the $\Gamma$ point, in analogy to the calculation presented for the $K$ point above. In addition to the honeycomb lattice of graphene with two atoms per unit cell, we have also calculated the corresponding Hamiltonians for a hexagonal and a quadratic lattice with one atom per unit cell. As the symmetry at the $\Gamma$ point is higher than at the $K$ point, we expect the set of allowed basis functions for the band dispersion to be smaller. The energy dispersion, which we have found from the tight-binding model presented here to second order in momentum $k$, is

$$E_\lambda(k) = \frac{\hbar^2}{2m}k^2 + \lambda_R|k| + E_0$$  \hfill (24)

with the origin of the momentum $k$ at the $\Gamma$ point. The projection given in Eq. (12) has been carried out at $\epsilon = \eta V_{pp\pi}$ with $\eta$ being the number of nearest neighbors in the respective lattice. The different coefficients in terms of the tight-binding parameters are

$$\frac{\hbar^2}{2m} = -\frac{1}{4}d^2\eta\left(V_{pp\pi} - \frac{2\xi^2}{V_{pp\pi} - V_{pp0}} + \frac{2\xi^2\eta\gamma_{sp1}(\gamma_{sp} + \gamma_{sp1})}{\eta V_{pp\pi} - \eta V_{ss0} - \epsilon_s}\right),$$

$$E_0 = \eta V_{pp\pi} + \frac{\alpha^2}{\eta V_{pp\pi} - \eta V_{pp0}} + \frac{\xi^2(\gamma_{sp} + \gamma_{sp1})^2}{\eta V_{pp\pi} - \eta V_{ss0} - \epsilon_s},$$

$$\alpha_R = \frac{d\alpha\xi\gamma_{pp1}}{V_{pp\pi} - V_{pp0}}.$$

Here, $d$ is the nearest-neighbor distance of the respective lattice. Because of the high symmetry at the $\Gamma$ point, the zeroth-order Rashba parameter $\alpha_R$ is zero so that the lowest-order contribution is the linear Rashba constant $\lambda_R$. It is equivalent to the phenomenological description of the nearest-neighbor Rashba term. The results for the different lattices (effective mass and energy offset) only differ from each other by the number of nearest neighbors involved, i.e., $\eta = 3$ for the honeycomb lattice, $\eta = 4$ for the hexagonal lattice, and $\eta = 6$ for the quadratic lattice. A schematic of the band dispersion is shown in Fig. 4. The characteristic offset can be clearly seen. Since $\Gamma$ is a time-reversal invariant point in the two-dimensional Brillouin zone, the spin-split band remains degenerate there. The atomic spin-orbit coupling strength $\alpha$ and the electric field $\xi$ introduce small corrections to the

![FIG. 3. (Color online) Dispersion of the graphene bands near the Fermi level at the $K$ point for different contributions from the potential gradient.](image1)

![FIG. 4. (Color online) Dispersion of a two-dimensional state at the $\Gamma$ point for different contributions from the potential gradient. The effective mass $m$ is 0.4 $m_e$ ($m_e$: free electron mass), the energy offset $E_0$ is zero, and the linear Rashba constant $\alpha_R$ is 0.33 eV Å.](image2)
effective mass and the energy offset. Interestingly, the linear Rashba constant $\alpha_R$ only depends on the electric field $\ell$ through the nearest-neighbor overlap of the $p_{xy}$ orbitals with the $p_z$ orbital in agreement with Petersen and Hedegård.\cite{2,18} It does not depend on the on-site contribution $g_{sp}$. Moreover, the linear Rashba constant $\alpha_R$ is independent of the details in the three lattices. This gives the result a certain kind of universality.

VII. APPLICATION TO A CORRUGATED LATTICE

Many systems with a sizable Rashba-type spin splitting have a corrugated surface structure (e.g., Bi, Sb, Ag, or Cu based surface alloys with Bi, Pb, Sb).\cite{19–25} The simplest approach to describe a corrugated surface is a honeycomb lattice where the two basis atoms are displaced by $\pm \Delta z$ from the $xy$ plane. This structure mimics the topmost surface layer of, e.g., the Bi(111) or Sb(111) surface. The linear Rashba constant $\alpha_R$ in a corrugated honeycomb lattice amounts to

$$\alpha_R = \frac{\alpha \xi V_{pp1}}{V_{pp1} - V_{pp0}}$$  \hspace{1cm} (26)

and is identical to the one for the uncorrugated lattice [see Eq. (25)]. It increases proportionally to the nearest-neighbor distance $d$. As the values of the tight-binding parameters decrease with increasing distance $d$ (see, e.g., Ref. 26), we expect a corresponding increase in the Rashba constant as well.

In the literature, a strong increase of the Rashba-type spin splitting due to the corrugation of the surface has been discussed extensively.\cite{25,27–30} In particular, for the Ag and Cu based surface alloys with Bi, Pb, or Sb, a correspondence between the outward relaxation of the alloy atoms and the strength of the Rashba-type spin splitting has been observed.\cite{29} However, for the tight-binding model presented here a corrugation of the lattice does not result in a particular enhancement of the Rashba-type spin splitting. Obviously, a more detailed model, possibly an inclusion of the $d$ bands\cite{3} or higher-order contributions to the Rashba coefficient,\cite{31} is needed to describe this enhancement by corrugation.

VIII. CONCLUSION

In summary, we have presented an extended $sp$-band tight-binding model for the Rashba-type spin splitting in two-dimensional lattices by combining the on-site and nearest-neighbor contributions from the potential gradient. Concerning the conical band structure near the $K$ point of graphene, it combines the effective on-site and nearest-neighbor Rashba terms [Eqs. (17) and (18)] along with other Rashba terms that are not included in the effective Rashba terms. The tight-binding model thus further validates the already successful phenomenological description at the same time pointing out that it is not complete. The nearest-neighbor contribution from the potential gradient gives a sizable contribution to the zeroth-order Rashba constant $\lambda_R$, as well as a nonzero linear Rashba constant $\alpha_R$. Hence both the on-site and the nearest-neighbor contribution should be considered in model calculations. At the $\Gamma$-point quadratic, hexagonal as well as flat and corrugated honeycomb lattices all give the same simple expression for the linear Rashba parameter $\alpha_R$, which only depends on the nearest-neighbor contribution from the potential gradient. In particular, it is independent of the details of the lattices giving the result a certain kind of universality and confirms the success of the phenomenological nearest-neighbor Rashba term.

In the next step would be to combine this model with the results from $d$-band contributions and higher-order contributions to the Rashba coefficient,\cite{31} which have been shown to add to the Rashba-type spin splitting. Successively including more components to this model will at the end lead to a better understanding of the Rashba-type spin splitting at surfaces.

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\begin{thebibliography}{9}
    \bibitem{18} In Ref. 2, the authors present an expression for the linear Rashba constant $\alpha_R$, which is slightly different from ours. We trace this back to a calculational error on their part. Furthermore, the nearest-neighbor distance $d$ does not enter in their calculation. Nevertheless, we believe that the main conclusions that can be drawn are the same.
\end{thebibliography}