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Eight-band $\mathbf{k}\cdot\mathbf{p}$ model of strained zinc-blende crystals

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Second-order Löwdin perturbation theory is used to calculate the interaction matrices for an eight-band $\mathbf{k}\cdot\mathbf{p}$ model (near the Γ point) of zinc-blende crystals under a uniform strain. The model treats the Γ_6 conduction bands, Γ_8 valence bands, and Γ_7 spin-orbit split-off bands. The model includes strain interactions arising from both the orbital and spin-orbit terms of the Hamiltonian. In addition to the usual Pikus-Bir deformation-potential constants, a, b, and d, which describe the coupling of the valence band to strain, two new deformation-potential constants arise, a' and b', which describe the coupling of the conduction band to strain. The constant a' couples the conduction band to hydrostatic deformations and the constant b', which results from a lack of inversion symmetry, couples the conduction band to shear deformations. The strain also introduces a $\mathbf{k}$-dependent conduction-band–valence-band mixing that is linear in strain, in wave vector, and in the momentum matrix element between the conduction and valence bands. In the absence of strain, the eight-band Kane model is recovered. Under a finite strain, in the limit of a large conduction-band–valence-band gap and large spin-orbit splitting, the four-band Luttinger model with strain is recovered.

I. INTRODUCTION

Theoretical[1–4] and experimental[5–9] work on strained Si and Ge crystals has been instrumental in gaining a detailed understanding of their energy-band structures. These crystals, which have an indirect energy gap in $\mathbf{k}$ space,[10] are characterized by a complex valence band, and consequently, many past research efforts concentrated on achieving a detailed understanding of valence-band mixing effects.

More recently, there is considerable interest in direct-gap zinc-blende semiconductors, such as GaAs and InSb, as well as strained-layer heterostructures because of their potential optoelectric applications.[11,12] Experiments dealing with strained zinc-blende bulk crystals[13,14] and strained-layer heterostructures[15–19] are interpreted using the Luttinger (four- or six-band) model for bulk crystals[20–22] with the strain interaction matrix derived by Pikus and Bir[1,2] or Suzuki and Hensel.[8] These models assume the diamond structure (O_h point group), which contains inversion as a symmetry operation, and treat the light-hole, heavy-hole, and spin-orbit split-off valence-band states, but they neglect the conduction band and the details of valence- and conduction-band mixing.

The purpose of this paper is to extend earlier work to include the strain-dependent coupling between the conduction and valence bands. We calculate the interaction matrices of a $\mathbf{k}\cdot\mathbf{p}$ model for strained zinc-blende crystals. The model treats the (Γ_6) conduction band, the (Γ_8) light- and heavy-hole bands, and the (Γ_7) spin-orbit split-off valence bands (T_d point group). The model includes certain strain interactions that have not been discussed by Pikus and Bir in their treatment of zinc-blende crystals.[2,23] We include in the model strain interactions coming from the orbital part of the Hamiltonian, as well as the largest portion of the strain interactions from the spin-orbit part of the Hamiltonian. The lack of inversion symmetry in zinc-blende crystals leads to certain mixing effects that are absent in the diamond structure.

When the conduction band is included together with the valence bands, there emerge two extra deformation-potential constants, a' and b', in addition to the deformation-potential constants[24] a, b, and d of Pikus-Bir.[1,2] The deformation-potential constant a' is the usual one that couples the conduction band to hydrostatic deformations. The lack of inversion symmetry in zinc blende gives rise to b', which induces a mixing of conduction and valence bands in the presence of shear deformations and results in a coupling of the conduction band to shear strains. Large shear strains are expected to exist in strained-layer heterostructures grown along the (111) crystal axis.[25] Experiments on such structures may be fruitful in determining values for this deformation-potential constant.[26] The strain interactions also induce mixing between conduction and valence bands through matrix elements that are linear in strain and in wave vector $\mathbf{k}$.

Our approach closely follows the works of Kane[27] and Pikus and Bir.[1,2] We use the transformation originally introduced by Pikus and Bir to obtain the strain interaction terms, but we treat these terms using Löwdin perturbation theory,[28] as was done by Kane in the absence of strain. This approach allows us to clearly see the origins of the strain couplings and the approximations made in their treatment using perturbation theory.

In order to clearly show all the approximations made in the eight-band model, we give a detailed derivation of the model in Sec. II. In Sec. III, we take a limiting case of the eight-band model to recover the four-band Luttinger model with strain interaction.

II. DERIVATION OF THE EIGHT-BAND MODEL WITH STRAIN

In the absence of strain, a zinc-blende crystal will have a lattice constant c_0 along the edges of the unit cell, defined by the orthonormal vectors $\hat{\mathbf{a}}_1$, $\hat{\mathbf{a}}_2$, and $\hat{\mathbf{a}}_3$. The band structure can be found by solving the $\mathbf{k}\cdot\mathbf{p}$ equation[27]

$$Hu_{n\mathbf{k}}^{(0)}(\mathbf{x})=E_n^{(0)}(\mathbf{k})u_{n\mathbf{k}}^{(0)}(\mathbf{x}) \ , \tag{1}$$

where

$$H=H_0+H_{\mathbf{k}}+H_{\mathbf{k}\cdot\mathbf{p}}+H_{\text{s.o.}}+H'_{\text{s.o.}} \tag{2}$$

and

$$H_0=\frac{\mathbf{p}^2}{2m_0}+V_0(\mathbf{x}) \ , \tag{2a}$$

$$H_{\mathbf{k}}=\frac{\hbar^2\mathbf{k}^2}{2m_0} \ , \tag{2b}$$

$$H_{\mathbf{k}\cdot\mathbf{p}}=\frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p} \ , \tag{2c}$$

$$H_{\text{s.o.}}=\frac{\hbar}{4m_0^2c^2}(\nabla V_0)\times\mathbf{p}\cdot\boldsymbol{\sigma} \ , \tag{2d}$$

$$H'_{\text{s.o.}}=\frac{\hbar^2}{4m_0^2c^2}(\nabla V_0)\times\mathbf{k}\cdot\boldsymbol{\sigma} \ , \tag{2e}$$

for the periodic Bloch spinor, $u_{n\mathbf{k}}^{(0)}(\mathbf{x})$. The potential $V_0(\mathbf{x})$ is the self-consistent periodic potential of the unstrained crystal, m_0 is the bare electron mass, and $\boldsymbol{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ are the Pauli spin matrices

$$\sigma_x=\begin{bmatrix}0&1\\1&0\end{bmatrix},\quad \sigma_y=\begin{bmatrix}0&-i\\i&0\end{bmatrix},\quad \sigma_z=\begin{bmatrix}1&0\\0&-1\end{bmatrix} . \tag{3}$$

The superscript on $u_{n\mathbf{k}}^{(0)}(\mathbf{x})$ is used to denote Bloch spinors in the unstrained crystal. Standard notation is used for the other quantities.

When the crystal is strained it has a new crystalline potential which can be denoted by $V(\mathbf{x};\overleftrightarrow{e})$, such that $V(\mathbf{x};\overleftrightarrow{e})\rightarrow V_0(\mathbf{x})$ when $\overleftrightarrow{e}\rightarrow 0$, where $\overleftrightarrow{e}$ is the strain dyadic with components e_{ij}. Under an arbitrary strain the periodicity of the crystal is destroyed and Bloch's theorem is invalid. However, for the case of a strain that is uniform in space, the potential $V(\mathbf{x},\overleftrightarrow{e})$ has a new periodicity,[1,2] with lattice constants c_1, c_2, and c_3, along the new axes, $\hat{\mathbf{a}}'_1$, $\hat{\mathbf{a}}'_2$, and $\hat{\mathbf{a}}'_3$. Under this strain a point initially at $\sum x_i\hat{\mathbf{a}}_i$ moves to a new position, $\sum x_i\hat{\mathbf{a}}'_i\equiv\sum x'_i\hat{\mathbf{a}}_i$, where the new (generally nonorthonormal) basis vectors $\hat{\mathbf{a}}'_1$, $\hat{\mathbf{a}}'_2$, and $\hat{\mathbf{a}}'_3$, are related to the original basis vectors by[29]

$$\hat{\mathbf{a}}'_i=\sum_j(\delta_{ij}+e_{ij})\hat{\mathbf{a}}_j \ . \tag{4}$$

The lattice constants with and without strain are related by

$$c_i=\left[1+\sum_j e_{ij}\right]c_0 \ . \tag{5}$$

The band structure in the presence of strain (for any $\mathbf{k}$ in the Brillouin zone) can be found by solving Eq. (1) with $V(\mathbf{x};\overleftrightarrow{e})$ in place of $V_0(\mathbf{x})$. However, the eigenspinors for this problem have a different spatial periodicity than the basis spinors in the unstrained crystal. Consequently, expanding the potential $V(\mathbf{x};\overleftrightarrow{e})$ in powers of e_{ij} and performing a direct perturbation expansion using the original unstrained crystal basis spinors is a poor approach. Instead we use the method of Pikus and Bir[1,2] by which we can restore the unstrained crystal periodicity to the eigenvalue problem. With $V(\mathbf{x};\overleftrightarrow{e})$ in place of $V_0(\mathbf{x})$, we transform Eq. (1), to a deformed coordinate system, x', using the transformation

$$x_i=\sum_j(\delta_{ij}+e_{ij})x'_j \ . \tag{6}$$

We can then perform a perturbation expansion in the deformed coordinates and transform back to the original coordinates.

For small strains the potential of the deformed crystal, $V(\mathbf{x};\overleftrightarrow{e})$, can be expanded to first order in the strain as

$$V(\mathbf{x};\overleftrightarrow{e})=V_0(\mathbf{x}')+\sum_{ij}V_{ij}(\mathbf{x}')e_{ij} \ , \tag{7}$$

where $V_{ij}(\mathbf{x}')=[\partial V(\mathbf{x}'+\overleftrightarrow{e}\cdot\mathbf{x}';\overleftrightarrow{e})/\partial e_{ij}]_{e_{ij}=0}$. The eigenvalue problem in the deformed coordinate system, correct to linear terms in the strain, can be written as

$$(H'+D)\tilde{u}_{n\mathbf{k}}(\mathbf{x}')=E_n(\mathbf{k})\tilde{u}_{n\mathbf{k}}(\mathbf{x}') \ , \tag{8}$$

where $\tilde{u}_{n\mathbf{k}}(\mathbf{x}')=u_{n\mathbf{k}}(\mathbf{x})$, and $u_{n\mathbf{k}}(\mathbf{x})$ is the solution to Eq. (1) with $V(\mathbf{x},\overleftrightarrow{e})$ in place of $V_0(\mathbf{x})$. The operator H' is the same as H, given by Eq. (2), but $\mathbf{x}$ and $\mathbf{p}$ are replaced by $\mathbf{x}'$ and $\mathbf{p}'$. The terms linear in strain,

$$D=D_0+D_{\mathbf{k}\cdot\mathbf{p}}+D_{\text{s.o.}}+D'_{\text{s.o.}} \ , \tag{9}$$

are functions of the operators $\mathbf{x}'$ and $\mathbf{p}'$ in the deformed coordinate system and are given by (with $\mathbf{x}'$ and $\mathbf{p}'$ replaced by $\mathbf{x}$ and $\mathbf{p}$)

$$D_0=\sum_{ij}\left[-\frac{1}{m_0}p_ip_j+V_{ij}(\mathbf{x})\right]e_{ij} \ , \tag{9a}$$

$$D_{\mathbf{k}\cdot\mathbf{p}}=-\frac{\hbar}{m_0}\mathbf{k}\cdot\overleftrightarrow{e}\cdot\mathbf{p} \ , \tag{9b}$$

$$\begin{aligned}D_{\text{s.o.}}=\frac{\hbar}{4m_0^2c^2}\Bigg[&\sum_{ij}e_{ij}[\nabla V_{ij}(\mathbf{x})]\times\mathbf{p}\cdot\boldsymbol{\sigma}\\&-[\nabla V_0(\mathbf{x})\cdot\overleftrightarrow{e}]\times\mathbf{p}\cdot\boldsymbol{\sigma}\\&-\nabla V_0(\mathbf{x})\times(\overleftrightarrow{e}\cdot\mathbf{p})\cdot\boldsymbol{\sigma}\Bigg] \ ,\end{aligned} \tag{9c}$$

$$\begin{aligned}D'_{\text{s.o.}}=\frac{\hbar^2}{4m_0^2c^2}\Bigg[&\sum_{ij}e_{ij}[\nabla V_{ij}(\mathbf{x})]\times\mathbf{k}\cdot\boldsymbol{\sigma}\\&-[\nabla V_0(\mathbf{x})\cdot\overleftrightarrow{e}]\times\mathbf{k}\cdot\boldsymbol{\sigma}\Bigg] \ .\end{aligned} \tag{9d}$$

The eigenvalue problem in Eq. (8) now contains the potential $V_0(\mathbf{x}')$, which has the periodicity of the unstrained crystal. In what follows we restrict ourselves to values of $\mathbf{k}$ near the Γ point. We use the basis spinors at $\mathbf{k}=0$ from the unstrained crystal, $v_n(\mathbf{x}')$ [given in Eq. (A2) of Appendix A], as basis spinors for doing a Löwdin perturbation[28] expansion in the deformed coordinate system x'. States v_n within the eight-dimensional manifold are taken to be in class A, while all other states are taken to be in class B. Second-order perturbation theory leads to the nonlinear eigenvalue problem[28]

$$\sum_{n=1}^{A} (U_{mn} - E\delta_{mn})C_n = 0 , \tag{10}$$

where $U_{mn} = \langle v_m | H(\mathbf{k}) + D(\mathbf{k}, \overleftrightarrow{\mathbf{e}}) | v_n \rangle$ is the renormalized interaction matrix among the class-A states, given to linear order in the strain by

$$\langle v_m | H(\mathbf{k}) + D(\mathbf{k}, \overleftrightarrow{\mathbf{e}}) | v_n \rangle = H'_{mn} + \sum_{\alpha}^{B} \frac{H'_{m\alpha} H'_{\alpha n}}{E - E_\alpha} + D_{mn} + \sum_{\alpha}^{B} \frac{H'_{m\alpha} D_{\alpha n} + D_{m\alpha} H'_{\alpha n}}{E - E_\alpha} , \tag{11}$$

where the matrix elements $H'_{mn} = \langle v_m | H' | v_n \rangle$, $E_\alpha = \langle v_\alpha | H' | v_\alpha \rangle$, and $H'_{m\alpha} = \langle v_m | H' | v_\alpha \rangle$, etc. In Eqs. (10) and (11) the labels m and n refer to matrix elements among the class-A basis states. The sums in (11) are only over states in class B, labeled by α. The operators $H(\mathbf{k})$ and $D(\mathbf{k}, \overleftrightarrow{\mathbf{e}})$ defined by Eq. (11) act only within the class-A states. The renormalized interaction matrix U_{mn} takes into account the effect of states in class B on the states in class A. The first two terms in (11), given by matrix elements of $H(\mathbf{k})$, describe the band structure in the absence of strain and lead to the Kane eight-band model,[27] plus several other terms. The effects of strain are described by the operator $D(\mathbf{k}, \overleftrightarrow{\mathbf{e}})$. In what follows we neglect the last term in Eq. (11), which renormalizes the matrix elements of U_{mn} by strain interactions that couple class-A and -B states.

Within the class-A states in Eq. (11), we make a unitary transformation to basis states u_j (see Appendix A),

$$u_j = \sum_{n}^{A} R_{jn} v_n , \tag{12}$$

which form a basis for the irreducible representations of the T_d double group. In this new basis, the strain-independent Kane piece of the interaction operator can be written as

$$\langle u_i | H(\mathbf{k}) | u_j \rangle = \sum_{m,n}^{A} (R^\dagger)_{mi} R_{jn} \left[\langle v_m | H_0 + H_\mathbf{k} + H_{\mathbf{k}\cdot\mathbf{p}} | v_n \rangle + \sum_{\alpha}^{B} \frac{\langle v_m | H_{\mathbf{k}\cdot\mathbf{p}} | v_\alpha \rangle \langle v_\alpha | H_{\mathbf{k}\cdot\mathbf{p}} | v_n \rangle}{E - E_\alpha} \right] + \langle u_i | H_{\text{s.o.}} + H'_{\text{s.o.}} | u_j \rangle , \tag{13}$$

where we have included the small interaction $H'_{\text{s.o.}}$. This interaction results in small linear $\mathbf{k}$ matrix elements that mix the conduction band (Γ_6) with both the light- and heavy-hole bands (Γ_8) and also with the spin-orbit split-off bands (Γ_7). The operators H_0 and $H_\mathbf{k}$ are diagonal in the basis v_n and hence do not contribute in the second order of perturbation, where only off-diagonal elements enter. In addition, two cross terms in the second order of perturbation, the first coming from the products of matrix elements of $H_{\mathbf{k}\cdot\mathbf{p}}$ with ($H_{\text{s.o.}} + H'_{\text{s.o.}}$), and the second coming from products of matrix elements of ($H_{\text{s.o.}} + H'_{\text{s.o.}}$) with itself, have been dropped. The first cross term leads to (small) linear and quadratic $\mathbf{k}$ terms. The linear $\mathbf{k}$ terms have been shown to be negligibly small.[27] The quadratic $\mathbf{k}$ terms, coming from products of matrix elements of $H_{\mathbf{k}\cdot\mathbf{p}}$ with $H'_{\text{s.o.}}$, are even smaller because $H'_{\text{s.o.}}$ is a much weaker interaction than $H_{\text{s.o.}}$, due to the smallness of $\hbar\mathbf{k}$ as compared with matrix elements of $\mathbf{p}$. The second cross term, containing products of matrix elements of $H_{\text{s.o.}}$ with itself, $H_{\text{s.o.}}$ with $H'_{\text{s.o.}}$, and $H'_{\text{s.o.}}$ with itself, leads to small $\mathbf{k}$-independent, linear, and quadratic $\mathbf{k}$ terms, respectively. All the above-mentioned terms arise from matrix elements that couple class-A and -B states, leading to corrections that are expected to be small for eigenvalues well within the class-A energy range. Following Kane we neglect these terms.[27]

The operator H_0 in Eq. (13) is diagonal in the basis v_n, with eigenvalues E_c and E'_v for the conduction- and valence-band states, respectively. The operators in the large parentheses in Eq. (13) are spin-independent, and consequently, the matrix within the large parentheses can be written as block diagonal,

$$\begin{bmatrix} \mathbf{H}_{\text{int}} & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_{\text{int}} \end{bmatrix} ,$$

where $\mathbf{H}_{\text{int}}$ is Kane's 4×4 interaction matrix[27] given by[30]

$$\begin{array}{cccc} s & x & y & z \\ \left[\begin{array}{c} E_c + A'k^2 + \hbar^2 k^2/2m_0 \\ \\ Bk_y k_z - iP_0 k_x \\ \\ Bk_x k_z - iP_0 k_y \\ \\ Bk_x k_y - iP_0 k_z \\ \end{array}\right. & \begin{array}{c} Bk_y k_z + iP_0 k_x \\ \\ E'_v + M(k_y^2 + k_z^2) \\ + L'k_x^2 + \hbar^2 k^2/2m_0 \\ N'k_x k_y \\ \\ N'k_x k_z \\ \end{array} & \begin{array}{c} Bk_x k_z + iP_0 k_y \\ \\ N'k_x k_y \\ \\ E'_v + M(k_x^2 + k_z^2) \\ + L'k_y^2 + \hbar^2 k^2/2m_0 \\ N'k_y k_z \\ \end{array} & \left.\begin{array}{c} Bk_x k_y + iP_0 k_z \\ \\ N'k_x k_z \\ \\ N'k_y k_z \\ \\ E'_v + M(k_x^2 + k_y^2) \\ + L'k_z^2 + \hbar^2 k^2/2m_0 \end{array}\right] \end{array} \tag{14}$$

Equation (14) is obtained by noting that all momentum matrix elements between the Γ_5 single group states vanish due to time reversal symmetry.[31] The Kane parameters A', B, P_0, M, N', and L' in (14) are taken to be constants by approximating the exact eigenvalue, E in Eq. (13), by conduction- and valence-band energies, E_c and E_v'. This approximation has the effect of linearizing the eigenvalue problem in Eq. (10). These constants can be determined experimentally or they can be calculated from their definitions given in Appendix B. The parameter P_0 mixes the conduction- and valence-band states away from $\mathbf{k}=0$. The parameter B is the inversion symmetry parameter. When $B=0$, the matrix in (14) corresponds to the diamond structure.

The spin-orbit interaction $H_{\text{s.o.}}$ transforms as Γ_1 and is diagonal in the double group basis class-A states u_j, taking the values 0, $\Delta/3$, and $-2\Delta/3$, for the Γ_6, Γ_8, and Γ_7 irreducible representations, respectively, where Δ is defined in Appendix B. In the new basis u_j, the interaction matrix in (13), $\langle u_i|H(\mathbf{k})|u_j\rangle$, *without* the $\mathbf{k}$-dependent spin-orbit matrix $\langle u_i|H'_{\text{s.o.}}|u_j\rangle$, is given by the following:

$$\begin{array}{cccccccc}
u^{\Gamma_6}_{-1/2} & u^{\Gamma_6}_{1/2} & u^{\Gamma_8}_{-3/2} & u^{\Gamma_8}_{-1/2} & u^{\Gamma_8}_{1/2} & u^{\Gamma_8}_{3/2} & u^{\Gamma_7}_{-1/2} & u^{\Gamma_7}_{1/2} \\
\end{array}$$

$$\left[\begin{array}{cccccccc}
A & 0 & T^*+V^* & 0 & -\sqrt{3}(T-V) & \sqrt{2}(W-U) & W-U & \sqrt{2}(T^*+V^*) \\
0 & A & \sqrt{2}(W-U) & -\sqrt{3}(T^*+V^*) & 0 & T-V & -\sqrt{2}(T-V) & W^*+U \\
T+V & \sqrt{2}(W^*-U) & -P+Q & -S^* & R & 0 & (\frac{3}{2})^{1/2}S & -\sqrt{2}Q \\
0 & -\sqrt{3}(T+V) & -S & -P-Q & 0 & R & -\sqrt{2}R & \frac{1}{\sqrt{2}}S \\
-\sqrt{3}(T^*-V^*) & 0 & R^* & 0 & -P-Q & S^* & \frac{1}{\sqrt{2}}S^* & \sqrt{2}R^* \\
\sqrt{2}(W^*-U) & T^*-V^* & 0 & R^* & S & -P+Q & \sqrt{2}Q & (\frac{3}{2})^{1/2}S^* \\
W^*-U & -\sqrt{2}(T^*-V^*) & (\frac{3}{2})^{1/2}S^* & -\sqrt{2}R^* & \frac{1}{\sqrt{2}}S & \sqrt{2}Q & Z & 0 \\
\sqrt{2}(T+V) & W+U & -\sqrt{2}Q & \frac{1}{\sqrt{2}}S^* & \sqrt{2}R & (\frac{3}{2})^{1/2}S & 0 & Z
\end{array}\right], \tag{15}$$

$$\begin{aligned}
A &= E_c + \left[A' + \frac{\hbar^2}{2m_0} \right](k_x^2+k_y^2+k_z^2) , \\
U &= \frac{1}{\sqrt{3}} P_0 k_z , \\
V &= \frac{1}{\sqrt{6}} P_0 (k_x - ik_y) , \\
W &= i\frac{1}{\sqrt{3}} B k_x k_y , \\
T &= \frac{1}{\sqrt{6}} B k_z (k_x + ik_y) , \\
P &= -E_v + \tfrac{1}{2}\gamma_1 \frac{\hbar^2}{m_0}(k_x^2+k_y^2+k_z^2) , \\
Q &= \tfrac{1}{2}\gamma_2 \frac{\hbar^2}{m_0}(k_x^2+k_y^2-2k_z^2) , \\
R &= -\frac{\sqrt{3}}{2}\left[\gamma_2 \frac{\hbar^2}{m_0}(k_x^2-k_y^2) - 2i\gamma_3 k_x k_y \right] , \\
S &= \sqrt{3}\gamma_3 \frac{\hbar^2}{m_0} k_z (k_x - ik_y) , \\
Z &= E_v - \Delta - \tfrac{1}{2}\gamma_1 \frac{\hbar^2}{m_0}(k_x^2+k_y^2+k_z^2) ,
\end{aligned} \tag{16}$$

and

$$E_v = E_v' + \frac{\Delta}{3} . \tag{16a}$$

The constants γ_1, γ_2, and γ_3 are the *modified* Luttinger parameters and are given in terms of the Kane parameters [see Eq. (B1) in Appendix B]:

$$\begin{aligned}
\gamma_1 &= -\frac{2}{3}\frac{m_0}{\hbar^2}(L'+2M) - 1 , \\
\gamma_2 &= -\frac{1}{3}\frac{m_0}{\hbar^2}(L'-M) , \\
\gamma_3 &= -\frac{1}{3}\frac{m_0}{\hbar^2}N' .
\end{aligned} \tag{17}$$

The *modified* Luttinger parameters are related[32] to the parameters used by Luttinger,[22] γ_1^L, γ_2^L, and γ_3^L, by

$$\begin{aligned}
\gamma_1 &= \gamma_1^L - \frac{E_P}{3E_g+\Delta} , \\
\gamma_2 &= \gamma_2^L - \frac{1}{2}\frac{E_P}{3E_g+\Delta} , \\
\gamma_3 &= \gamma_3^L - \frac{1}{2}\frac{E_P}{3E_g+\Delta} ,
\end{aligned} \tag{18}$$

where

$$E_g = E_c - E_v , \tag{18a}$$

and E_P, a parameter that controls mixing of the valence and conduction bands, is related to P_0 by

$$E_P=\frac{2m_0}{\hbar^2}P_0^2\ . \tag{19}$$

In Eq. (16) the constant A' results from the interaction of the Γ_6 conduction band with class-B states [see Eq. (B1)].

The matrix elements of the **k**-dependent spin-orbit interaction in Eq. (13) are given by

$$\langle u_i|H'_{\text{s.o.}}|u_j\rangle=\begin{array}{c}\begin{array}{ccc}\Gamma_6 & \Gamma_8 & \Gamma_7\end{array}\\ \left[\begin{array}{ccc}0 & \mathbf{M}_1 & \mathbf{M}_2\\ \mathbf{M}_1^\dagger & 0 & 0\\ \mathbf{M}_2^\dagger & 0 & 0\end{array}\right]\end{array}\ , \tag{20}$$

where the 2×4 matrix $\mathbf{M}_1$ and the 2×2 matrix $\mathbf{M}_2$ are given by

$$\mathbf{M}_1=\frac{C_0}{\sqrt{2}}\begin{array}{c}\begin{array}{cccc}u_{-3/2}^{\Gamma_8} & u_{-1/2}^{\Gamma_8} & u_{1/2}^{\Gamma_8} & u_{3/2}^{\Gamma_8}\end{array}\\ \left[\begin{array}{cccc}-(k_x+ik_y) & 0 & -\sqrt{3}(k_x-ik_y) & 2k_z\\ 2k_z & \sqrt{3}(k_x+ik_y) & 0 & k_x-ik_y\end{array}\right]\end{array}\ , \tag{21}$$

$$\mathbf{M}_2=2C_0\begin{array}{c}\begin{array}{cc}u_{-1/2}^{\Gamma_7} & u_{1/2}^{\Gamma_7}\end{array}\\ \left[\begin{array}{cc}-k_z & k_x+ik_y\\ k_x-ik_y & k_z\end{array}\right]\end{array}\ , \tag{22}$$

where

$$C_0=\frac{1}{\sqrt{3}}\frac{\hbar^2}{4m_0^2c^2}\left\langle s\left|\frac{\partial V_0}{\partial x}\right|x\right\rangle\ . \tag{23}$$

To obtain Eqs. (20)–(23) we have made use of the fact that the matrix element[2] $\langle x|(\partial V_0/\partial x)|z\rangle=0$. In the absence of strain, the total interaction matrix in Eq. (13), $\langle u_i|H(\mathbf{k})|u_j\rangle$, is given by the sum of the matrices in Eqs. (15) and (20). The constants A', B, P_0, γ_1, γ_2, γ_3, C_0, together with the band gap E_g and spin-orbit splitting Δ determine the band structure in the absence of strain.

The elements of the strain-dependent interaction operator $D(\mathbf{k},\overleftrightarrow{\epsilon})$ in the basis u_j can be written as

$$\langle u_i|D(\mathbf{k},\overleftrightarrow{\epsilon})|u_j\rangle=\sum_{m,n=1}^{A}(R^\dagger)_{mi}R_{jn}\langle v_m|D_0+D_{\mathbf{k}\cdot\mathbf{p}}|v_n\rangle+\langle u_i|D_{\text{s.o.}}+D'_{\text{s.o.}}|u_j\rangle\ , \tag{24}$$

where interactions which couple class-A and -B states in the second order of perturbation theory have been dropped. In the basis v_n, the operator $D_0+D_{\mathbf{k}\cdot\mathbf{p}}$ is spin independent and consequently can be written as a block-diagonal matrix,

$$\left[\begin{array}{cc}\overline{\mathbf{D}} & 0\\ 0 & \overline{\mathbf{D}}\end{array}\right]\ ,$$

where the 4×4 matrix $\overline{\mathbf{D}}$ is given by

$$\begin{array}{cccc} s & x & y & z\\ \left[\begin{array}{c} a'(e_{xx}+e_{yy}+e_{zz})\\ b'e_{yz}+iP_0\sum\limits_j e_{xj}k_j\\ b'e_{xz}+iP_0\sum\limits_j e_{yj}k_j\\ b'e_{xy}+iP_0\sum\limits_j e_{zj}k_j\end{array}\right. & \begin{array}{c} b'e_{yz}-iP_0\sum\limits_j e_{xj}k_j\\ le_{xx}+m(e_{yy}+e_{zz})\\ ne_{xy}\\ ne_{xz}\end{array} & \begin{array}{c} b'e_{xz}-iP_0\sum\limits_j e_{yj}k_j\\ ne_{xy}\\ le_{yy}+m(e_{xx}+e_{zz})\\ ne_{yz}\end{array} & \left.\begin{array}{c} b'e_{xy}-iP_0\sum\limits_j e_{zj}k_j\\ ne_{xz}\\ ne_{yz}\\ le_{zz}+m(e_{xx}+e_{yy})\end{array}\right]\end{array}\ , \tag{25}$$

$$\begin{aligned} a'&=\langle s|D_{xx}|s\rangle\ ,\\ b'&=2\langle s|D_{xy}|z\rangle\ ,\\ l&=\langle x|D_{xx}|x\rangle\ ,\\ m&=\langle y|D_{xx}|y\rangle\ ,\\ n&=2\langle x|D_{xz}|z\rangle\ ,\end{aligned} \tag{26}$$

and where D_{xy} is the x,y component of the operator D_{ij}, defined by writing D_0 in Eq. (9a) as

$$D_0=\sum_{ij}D_{ij}e_{ij}\ . \tag{27}$$

To obtain (25) we have used the fact that D_0 is a real Hermitian operator and that the basis functions s, x, y, and z can be chosen to be real because of time reversal symmetry.[20] The lower-right 3×3 block of the matrix in (25), containing the real constants l, m, and n, is identical to the matrix of Pikus and Bir, which describes the orbital valence-band strain interaction in the diamond structure.[1,2] The strain interaction operator $D_{\mathbf{k}\cdot\mathbf{p}}$, in the first-order perturbation, leads to the matrix elements in Eq. (25) that are linear in $\mathbf{k}$. These terms occur because strain reduces the crystal symmetry, leading to additional conduction-band–valence-band mixing through the momentum matrix element, P_0, between the conduction and valence bands.

These terms couple the conduction and valence bands when shear is present, as well as when uniaxial deformations are present along any of the crystal axis. The first row and column in (25) contain the deformation-potential constants a' and b', which describe the conduction-band strain interaction. The constant a' describes the coupling to hydrostatic deformations and the constant b' describes the coupling to shear deformations. In the case of the diamond structure where the Γ-point conduction-band states transform as Γ_2^- and the valence-band states transform as Γ_5^+ of the O_h group,[10] the shear deformation-potential constant b' is zero because of inversion symmetry.

In the eight-dimensional spinor basis u_j, the orbital part of the strain interaction matrix in Eq. (24), $\langle u_i|D_0+D_{\mathbf{k}\cdot\mathbf{p}}|u_j\rangle$, is given by

$$\left[\begin{array}{cccccccc}
u^{\Gamma_6}_{-1/2} & u^{\Gamma_6}_{1/2} & u^{\Gamma_8}_{-3/2} & u^{\Gamma_8}_{-1/2} & u^{\Gamma_8}_{1/2} & u^{\Gamma_8}_{3/2} & u^{\Gamma_7}_{-1/2} & u^{\Gamma_7}_{1/2} \\
a'e & 0 & t^*-v^* & 0 & -\sqrt{3}(t+v) & \sqrt{2}(w+u) & w+u & \sqrt{2}(t^*-v^*) \\
0 & a'e & \sqrt{2}(w+u) & -\sqrt{3}(t^*-v^*) & 0 & t+v & -\sqrt{2}(t+v) & w^*-u \\
t-v & \sqrt{2}(w^*+u) & -p+q & -s^* & r & 0 & (\frac{3}{2})^{1/2}s & -\sqrt{2}q \\
0 & -\sqrt{3}(t-v) & -s & -p-q & 0 & \mathrm{r} & -\sqrt{2}r & \frac{1}{\sqrt{2}}s \\
-\sqrt{3}(t^*+v^*) & 0 & r^* & 0 & -p-q & s^* & \frac{1}{\sqrt{2}}s^* & \sqrt{2}r^* \\
\sqrt{2}(w^*+u) & t^*+v^* & 0 & r^* & s & -p+q & \sqrt{2}q & (\frac{3}{2})^{1/2}s^* \\
w^*+u & -\sqrt{2}(t^*+v^*) & (\frac{3}{2})^{1/2}s^* & -\sqrt{2}r^* & \frac{1}{\sqrt{2}}s & \sqrt{2}q & -ae & 0 \\
\sqrt{2}(t-v) & w-u & -\sqrt{2}q & \frac{1}{\sqrt{2}}s^* & \sqrt{2}r & (\frac{3}{2})^{1/2}s & 0 & -ae
\end{array}\right] \tag{28}$$

where

$$w=i\frac{1}{\sqrt{3}}b'e_{xy},\quad p=a(e_{xx}+e_{yy}+e_{zz}),$$

$$t=\frac{1}{\sqrt{6}}b'(e_{xz}+ie_{yz}),\quad q=b[e_{zz}-\tfrac{1}{2}(e_{xx}+e_{yy})],$$

$$u=\frac{1}{\sqrt{3}}P_0\sum_j e_{zj}k_j,\quad r=\frac{\sqrt{3}}{2}b(e_{xx}-e_{yy})-ide_{xy}, \tag{29}$$

$$v=\frac{1}{\sqrt{6}}P_0\sum_j(e_{xj}-ie_{yj})k_j,\quad s=-d(e_{xz}-ie_{yz}),$$

$$e=e_{xx}+e_{yy}+e_{zz}.$$

The deformation-potential constants a, b, d, a', and b' contained in (28) couple the energy bands to the strain. The constants a' and b' are defined by the matrix elements given in Eq. (26). The Pikus-Bir deformation-potential constants a, b, and d are related to the matrix elements l, m, and n in Eq. (26) by

$$a=\tfrac{1}{3}(l+2m),$$

$$b=\tfrac{1}{3}(l-m), \tag{30}$$

$$d=\frac{1}{\sqrt{3}}n.$$

These constants can be calculated from their definitions or they can be determined from experiments. The linear $\mathbf{k}$ terms, u and v, in Eq. (28) come from the interaction $D_{\mathbf{k}\cdot\mathbf{p}}$, see Eq. (24).

The strain interactions $D_{\text{s.o.}}$ and $D'_{\text{s.o.}}$, coming from the spin-orbit interaction, are small. Since typical values of interest for $\hbar|\mathbf{k}|$ are 2 orders of magnitude smaller than the momentum matrix elements, we expect that the matrix elements of $D'_{\text{s.o.}}$ are 2 orders of magnitude smaller than the elements of $D_{\text{s.o.}}$. Consequently we neglect the matrix $\langle u_i|D'_{\text{s.o.}}|u_j\rangle$ in Eq. (24). The operator $D_{\text{s.o.}}$ can be written as

$$D_{\text{s.o.}}=D^{(0)}_{\text{s.p.}}+D^{(1)}_{\text{s.o.}}+D^{(2)}_{\text{s.o.}}, \tag{31}$$

where the three terms in (31) are defined in the order given in Eq. (9c). The operator $D^{(0)}_{\text{s.o.}}$ is Hermitian, while each of the operators $D^{(1)}_{\text{s.o.}}$ and $D^{(2)}_{\text{s.o.}}$ are separately not Hermitian, however the sum $D^{(1)}_{\text{s.o.}}+D^{(2)}_{\text{s.o.}}$ is a Hermitian operator. Rough estimates of the matrix elements among class-A states lead to the conclusion that $D^{(1)}_{\text{s.o.}}$ and $D^{(2)}_{\text{s.o.}}$ are of the same order of magnitude, but that $D^{(0)}_{\text{s.o.}}$ is 4 orders of magnitude smaller. Consequently, we will neglect[33] the interaction $D^{(0)}_{\text{s.o.}}$. The matrix elements of $D^{(1)}_{\text{s.o.}}+D^{(2)}_{\text{s.o.}}$ are given by [with basis functions arranged in the same order as in Eqs. (15) and (28)]

$$\langle u_i|D^{(1)}_{\text{s.o.}}+D^{(2)}_{\text{s.o.}}|u_j\rangle=\begin{array}{c}\begin{array}{ccc}\Gamma_6 & \Gamma_8 & \Gamma_7\end{array}\\ \left[\begin{array}{ccc} 0 & 0 & 0 \\ 0 & \mathbf{N}_1 & \mathbf{N}_2 \\ 0 & \mathbf{N}_2^\dagger & \mathbf{N}_3 \end{array}\right]\end{array}, \tag{32}$$

where the 4×4 matrix $\mathbf{N}_1$, the 4×2 matrix $\mathbf{N}_2$, and the 2×2 matrix $\mathbf{N}_3$ are given by

$$\mathbf{N}_1=\frac{\Delta}{3}\begin{bmatrix} e & -\frac{2}{\sqrt{3}}(e_{xz}+ie_{yz}) & i\frac{2}{\sqrt{3}}e_{xy} & 0 \\ -\frac{2}{\sqrt{3}}(e_{xz}-ie_{yz}) & e & 0 & i\frac{2}{\sqrt{3}}e_{xy} \\ -i\frac{2}{\sqrt{3}}e_{xy} & 0 & e & \frac{2}{\sqrt{3}}(e_{xz}+ie_{yz}) \\ 0 & -i\frac{2}{\sqrt{3}}e_{xy} & \frac{2}{\sqrt{3}}(e_{xz}-ie_{yz}) & e \end{bmatrix}, \tag{33}$$

$$\mathbf{N}_2=\frac{\Delta}{3}\begin{bmatrix} -(e_{xz}-ie_{yz}) & -\frac{1}{3\sqrt{2}}(3e_{zz}-e) \\ \frac{1}{\sqrt{6}}(e_{xx}-e_{yy}+i2\sqrt{2}e_{xy}) & -\frac{1}{\sqrt{3}}(e_{xz}-ie_{yz}) \\ -\frac{1}{\sqrt{3}}(e_{xz}+ie_{yz}) & -\frac{1}{\sqrt{6}}(e_{xx}-e_{yy}-i2\sqrt{2}e_{xy}) \\ \frac{1}{3\sqrt{2}}(3e_{zz}-e) & -(e_{xz}+ie_{yz}) \end{bmatrix}, \tag{34}$$

$$\mathbf{N}_3=\frac{\Delta}{3}\begin{bmatrix} -2e & 0 \\ 0 & -2e \end{bmatrix}. \tag{35}$$

We therefore find that in first order of perturbation theory the spin-orbit interactions $D^{(1)}_{\text{s.o.}}$ and $D^{(2)}_{\text{s.o.}}$ lead to matrix elements which couple the valence bands to both uniaxial and shear strains, through the spin-orbit splitting parameter Δ. Also, these interactions mix the light- and heavy-hole bands with the spin-orbit split-off bands by the matrix $\mathbf{N}_2$. However, these interactions have no effect on the conduction bands because they do not couple them to the valence bands.

The strain interaction matrix in Eq. (24), $\langle u_i|D(\mathbf{k},\overleftrightarrow{\mathbf{e}})|u_j\rangle$, is then approximately given by the sum of the matrices in Eqs. (28) and (32).

Due to time reversal symmetry the eigenvalues of U_{mn} satisfy $E_n(\mathbf{k})=E_n(-\mathbf{k})$. However, because of a lack of inversion symmetry the eigenvalues are not in general doubly degenerate (except along high-symmetry directions).

Transforming from the deformed coordinate system back to the original coordinate system, the Bloch functions of the deformed crystal are given by [see Eq. (8)]

$$u_{n\mathbf{k}}(\mathbf{x})=\sum_{j=1}^{A}B_j^{(n)}(\mathbf{k},\overleftrightarrow{\mathbf{e}})u_j(\mathbf{x}-\overleftrightarrow{\mathbf{e}}\cdot\mathbf{x}) , \tag{36}$$

where $n=1,\ldots,8$ labels the energy bands and $B_j^{(n)}(\mathbf{k},\overleftrightarrow{\mathbf{e}})$ is the jth component of the nth eigenvector of

$$\sum_{n=1}^{A}(U_{ij}-E\delta_{ij})B_j=0 , \tag{37}$$

where

$$U_{ij}=\langle u_i|H(\mathbf{k})+D(\mathbf{k},\overleftrightarrow{\mathbf{e}})|u_j\rangle . \tag{38}$$

III. THE LUTTINGER MODEL WITH STRAIN

The Luttinger four-band model is found from the eight-band model by taking the asymmetry parameter $B=0$, and taking the band gap, $E_g\equiv E_c-E_v$, and the spin-orbit splitting, Δ, to be arbitrarily large. The central 4×4 block of U_{ij} in Eq. (38) decouples and we must diagonalize the Luttinger (Γ_8) piece of the interaction matrix,

$$\mathbf{H}_{\text{Lutt}}=\mathbf{H}_0+\mathbf{H}_{\text{strain-orb}}+\mathbf{H}_{\text{strain-s.o.}} , \tag{39}$$

where

$$\mathbf{H}_0=-\begin{bmatrix} P-Q & S^* & -R & 0 \\ S & P+Q & 0 & -R \\ -R^* & 0 & P+Q & -S^* \\ 0 & -R^* & -S & P-Q \end{bmatrix}, \tag{40}$$

$$\mathbf{H}_{\text{strain-orb}}=-\begin{bmatrix} p-q & s^* & -r & 0 \\ s & p+q & 0 & -r \\ -r^* & 0 & p+q & -s^* \\ 0 & -r^* & -s & p-q \end{bmatrix}, \tag{41}$$

and $\mathbf{H}_{\text{strain-s.o.}}=\mathbf{N}_1$, where $\mathbf{N}_1$ is given in Eq. (33). The parameters p, q, r, and s that enter into Eq. (41) are defined in Eq. (29). However, the parameters P, Q, R, and S in Eq. (40) are *not* the same as those given in Eq. (16). The parameters P, Q, R, and S that enter in Eq. (40) are defined by

$$\begin{aligned} P&=\tfrac{1}{2}\gamma_1^L\frac{\hbar}{m_0}(k_x^2+k_y^2+k_z^2) , \\ Q&=-\tfrac{1}{2}\gamma_2^L\frac{\hbar}{m_0}(2k_z^2-k_x^2-k_y^2) , \\ R&=-\frac{\sqrt{3}}{2}\frac{\hbar}{m_0}[\gamma_2^L(k_x^2-k_y^2)-2i\gamma_3^Lk_xk_y] , \\ S&=\sqrt{3}\gamma_3^L\frac{\hbar}{m_0}k_z(k_x-ik_y) , \end{aligned} \tag{42}$$

where we have set the energy of the edge of the valence band, E_v, to zero. These parameters contain the Luttinger parameters, γ_1^L, γ_2^L, γ_3^L, and not the modified Luttinger parameters, γ_1, γ_2, γ_3, see Eq. (18).

IV. CONCLUSION

We have used Löwdin perturbation theory to calculate the interaction matrices for an eight-band **k·p** model of strained zinc-blende crystals. Our main results are given by Eqs. (28) and (32) which describe the strain-dependent coupling between the conduction and valence bands. The strain-dependent band structure near the Γ point can be calculated by diagonalizing the sum of the matrices in Eqs. (15), (20), (28), and (32). By including the conduction band on an equal footing with the valence bands we have found that in zinc-blende crystals two deformation-potential constants, a' and b', describe the coupling of the conduction band to strain. The constant a' is the coupling to hydrostatic deformations[23] while the constant b' results from the lack of inversion symmetry in zinc blende and couples the conduction band to shear deformations. Large shear deformations are expected to exist in (111) growth-axis heterostructures. Additionally, strain breaks the crystal symmetry which leads to additional mixing of the conduction and valence bands by terms that are linear in strain, in wave vector, and in the momentum matrix elements between conduction and valence bands [see the terms u and v in Eqs. (28) and (29)]. The interaction matrices derived above can be used within an effective-mass picture to study strained-layer heterostructures. This work is currently in progress.

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APPENDIX A: BASIS FUNCTIONS

We build up a basis from purely spatial eigenfunctions $u_{nj}^{\Gamma}(\mathbf{x}) \equiv \langle \mathbf{x} | n\Gamma j \rangle$, that satisfy

$$H_0 u_{nj}^{\Gamma}(\mathbf{x}) = E_{n,\Gamma} u_{nj}^{\Gamma}(\mathbf{x}) , \tag{A1}$$

where H_0 is given by Eq. (2a) in the text. The label Γ specifies the irreducible representation of the T_d single group, j labels the row to which the function belongs, and n specifies the band. Because of time reversal symmetry we are allowed to take these functions to be real[20,31] and we make use of this simplification. From the single group states $|n\Gamma j\rangle$, we take for the conduction band the s-like spatial function, $|s\rangle$, as a basis for the identity representation Γ_1, and for the valence band we take the p-like functions $|x\rangle$, $|y\rangle$, and $|z\rangle$ as a basis for the irreducible representation Γ_5. These states have the eigenenergies E_c and E_v' for the conduction and valence bands, respectively. In order to include electron spin we introduce the two eigenspinors of the operator σ_z,

$$\chi_\uparrow = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad \chi_\downarrow = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

which form a basis for Γ_6. We form a basis for the double group from the products $|n\Gamma j\rangle\chi_\uparrow$ and $|n\Gamma j\rangle\chi_\downarrow$. The states

$$\begin{aligned} v_1 &= |s\rangle\chi_\uparrow, & v_5 &= |s\rangle\chi_\downarrow , \\ v_2 &= |x\rangle\chi_\uparrow, & v_6 &= |x\rangle\chi_\downarrow , \\ v_3 &= |y\rangle\chi_\uparrow, & v_7 &= |y\rangle\chi_\downarrow , \\ v_4 &= |z\rangle\chi_\uparrow, & v_8 &= |z\rangle\chi_\downarrow , \end{aligned} \tag{A2}$$

will form the Löwdin class-A states. All other states of the form $|n\Gamma j\rangle\chi_\downarrow$ and $|n\Gamma j\rangle\chi_\uparrow$, which are not included in Eq. (A2), are class-B states. Using the Clebsch-Gordan coupling coefficients,[30] we make a unitary transformation within the class-A states to basis functions for the Γ_6, Γ_7, and Γ_8 irreducible representations of the T_d double group:

$$\begin{aligned} u_{-1/2}^{\Gamma_6} &= |s\rangle\chi_\downarrow , \\ u_{1/2}^{\Gamma_6} &= |s\rangle\chi_\uparrow , \\ u_{-3/2}^{\Gamma_8} &= \frac{-i}{\sqrt{6}}(|x\rangle + i|y\rangle)\chi_\downarrow + i\sqrt{\tfrac{2}{3}}|z\rangle\chi_\uparrow , \\ u_{-1/2}^{\Gamma_8} &= \frac{i}{\sqrt{2}}(|x\rangle + i|y\rangle)\chi_\uparrow , \\ u_{1/2}^{\Gamma_8} &= \frac{-i}{\sqrt{2}}(|x\rangle - i|y\rangle)\chi_\downarrow , \\ u_{3/2}^{\Gamma_8} &= \frac{i}{\sqrt{6}}(|x\rangle - i|y\rangle)\chi_\uparrow + i\sqrt{\tfrac{2}{3}}|z\rangle\chi_\downarrow , \\ u_{-1/2}^{\Gamma_7} &= \frac{-i}{\sqrt{3}}(|x\rangle - i|y\rangle)\chi_\uparrow + \frac{i}{\sqrt{3}}|z\rangle\chi_\downarrow , \\ u_{1/2}^{\Gamma_7} &= \frac{-i}{\sqrt{3}}(|x\rangle + i|y\rangle)\chi_\downarrow - \frac{i}{\sqrt{3}}|z\rangle\chi_\uparrow . \end{aligned} \tag{A3}$$

The states in (A3) satisfy the convention that under the time reversal operator

$$T = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} K , \tag{A4}$$

where K is complex conjugation, they transform as $Tu_i^{\Gamma} = (-1)^{q-i} u_{-i}^{\Gamma}$, where q is the maximum value of i for the irreducible representation Γ. In the text the spinors in Eqs. (A2) and (A3) are denoted by v_n and u_j, respectively, where the indices $n, j = 1, 2, \ldots, 8$, are used to label these spinors in the sequence given in Eqs. (A2) and (A3).

By construction, the spin-orbit interaction $H_{\text{s.o.}}$ is diagonal in the class-A states in Eq. (A3). However, $H_{\text{s.o.}}$ has nonzero matrix elements between the class-A and -B states. One can choose a different basis (also labeled by the Γ_6, Γ_8, and Γ_7 irreducible representations of the T_d double group) in which $H_0 + H_{\text{s.o.}}$ is diagonal. In this basis, the class-A states are mixtures of states given in Eq. (A3) and higher-lying states. A convenient aspect of this basis is that all the (strain-independent) linear **k** terms (some of which were discussed by Kane[27]), occur in the first order of perturbation theory from matrix elements of **k·p** and $H_{\text{s.o.}}'$. However, in this basis matrix elements of the momentum operator among the valence-band states are no longer zero.

APPENDIX B: DEFINITIONS OF THE CONSTANTS

The Kane parameters that enter into Eq. (16) are defined by

$$
\begin{aligned}
A' &= \frac{\hbar^2}{m_0^2} \sum_{nj} \frac{|\langle s|p_x|n\Gamma_5 j\rangle|^2}{E_c - E_{n,\Gamma_5}} , \\
B &= 2\frac{\hbar^2}{m_0^2} \sum_{nj} \frac{\langle s|p_x|n\Gamma_5 j\rangle\langle n\Gamma_5 j|p_x|z\rangle}{(E_c+E_v)/2 - E_{n,\Gamma_5}} , \\
M &= H_1 + H_2 , \\
L' &= F' + 2G , \\
N' &= F' - G + H_1 - H_2 , \\
P_0 &= -i\frac{\hbar}{m_0}\langle s|p_x|x\rangle , \\
\frac{\Delta}{3} &= -i\frac{\hbar}{4m_0^2c^2}\langle x|(\nabla V_0 \times \mathbf{p})_y|z\rangle , \\
G &= \frac{\hbar^2}{2m_0^2} \sum_{nj} \frac{|\langle x|p_x|n\Gamma_3 j\rangle|^2}{E_v - E_{n,\Gamma_3}} , \\
F' &= \frac{\hbar^2}{m_0^2} \sum_{nj} \frac{|\langle x|p_x|n\Gamma_1 j\rangle|^2}{E_v - E_{n,\Gamma_1}} , \\
H_1 &= \frac{\hbar^2}{2m_0^2} \sum_{nj} \frac{|\langle x|p_x|n\Gamma_5 j\rangle|^2}{E_v - E_{n,\Gamma_5}} , \\
H_2 &= \frac{\hbar^2}{2m_0^2} \sum_{nj} \frac{|\langle x|p_x|n\Gamma_4 j\rangle|^2}{E_v - E_{n,\Gamma_4}} .
\end{aligned}
\tag{B1}
$$

The sums in Eq. (B1) are over all single group states, $|n\Gamma j\rangle$, of the specified irreducible representation, excluding the states in the four-dimensional manifold, $|s\rangle$, $|x\rangle$, $|y\rangle$, and $|z\rangle$.

The parameters that enter into the Luttinger model,[22] γ_1^L, γ_2^L, and γ_3^L, are related to the Dresselhaus[20] parameters L, M, and N, by

$$
\begin{aligned}
\gamma_1^L &= -\frac{2}{3}\frac{m_0}{\hbar^2}(L+2M) - 1 , \\
\gamma_2^L &= -\frac{1}{3}\frac{m_0}{\hbar^2}(L-M) , \\
\gamma_3^L &= -\frac{1}{3}\frac{m_0}{\hbar^2}N .
\end{aligned}
\tag{B2}
$$

The Dresselhaus[20] parameters L, N, and F are related to the Kane parameters by

$$
\begin{aligned}
L &= F + 2G , \\
N &= F - G + H_1 - H_2 ,
\end{aligned}
\tag{B3}
$$

where

$$F = F' + \frac{P_0^2}{E_v' - E_c} .$$

The Dresselhaus parameters differ from the related Kane parameters L', N', and F' because Dresselhaus chose the three states labeled by x, y, and z as a basis for his manifold, rather than the four states s, x, y, and z used by Kane.[27]

APPENDIX C: NOTATIONS FOR T_d DOUBLE-GROUP IRREDUCIBLE REPRESENTATIONS

We present the following notations.

Parmenter[34]	Dresselhaus[31] Bir and Pikus[1,2]	KDWS (Ref. 12)
Γ_1	Γ_1	Γ_1
Γ_2	Γ_2	Γ_2
Γ_{12}	Γ_3	Γ_3
Γ_{15}	Γ_4	Γ_5
Γ_{25}	Γ_5	Γ_4
Γ_6	Γ_6	Γ_6
Γ_7	Γ_7	Γ_7
Γ_8	Γ_8	Γ_8

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[30] We evaluate matrix elements by expanding the interactions in irreducible tensors of the T_d double group and then we use the Wigner-Eckart theorem; see, for example, J. F. Cornwell, *Group Theory in Physics* (Academic, New York, 1984), Vol. I.

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