Analytical descriptions of the band structure of direct-band-gap zinc-blende-structure semiconductors in the k·p Kane model

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(Received 11 December 1990)

In the framework of the well-known **k·p** Kane band theory, accurate analytical approximations of conduction- and valence-band dispersion of direct-band-gap zinc-blende-structure semiconductors are derived when the spin-orbit-splitting energy does not exceed the band-gap energy. These approximations include the interactions with the remote bands. The expressions of the eigenfunctions are also obtained. The present analysis elucidates and unifies previous analytical band descriptions.

I. INTRODUCTION

The Kane **k·p** perturbation model[1] is widely used as a convenient way to describe the band structure of III-V semiconductor compounds. However the diagonalization of the **k·p** Hamiltonian leads to the resolution of a cubic equation, which does not yield simple expressions of the roots. Therefore, in the past, simple analytical band descriptions were derived, either around the zone center,[1] possibly accounting for the band nonparabolicity,[2] or at large wave-vector limits.[3] Empirical formulations of the conduction-band dispersion have also been given[4,5] and an alternative model, with convenient analytical solutions, has been developed but at the sacrifice of accuracy.[6] These approximations were used in transport calculations,[4,5] in the study of electron-spin relaxation or to analyze electron-spin polarization under optical pumping conditions.[3,6–8] More recently, Rode's expressions[4] have been rediscovered to discuss "universal" conduction-band-structure effects.[9] In the present paper, we analytically derive simple algebraic expressions of the conduction- and valence-band dispersions in the framework of the Kane model. These approximate solutions are accurate when the spin-orbit-splitting energy Δ does not exceed the band gap energy E_G. Our treatment also relates the above-mentioned approaches to the Kane theory.

II. THE KANE MODEL

In the **k·p** Kane theory[1] the **k·p** perturbation and the spin-orbit interaction are exactly diagonalized in the quasidegenerate band subset formed by the first conduction band, the heavy-hole band, the light-hole band, and the spin-orbit-split band, hereafter referred to as Γ_6, Γ_{8h}, Γ_{8l}, and Γ_7 bands. The energy origin is taken at the top of the valence band. The four double roots of the resulting secular equation are given by

$$\varepsilon'=0 , \tag{1}$$

$$(\varepsilon'-E_G)\varepsilon'(\varepsilon'+\Delta)-(k\mathcal{P})^2(\varepsilon'+2\Delta/3)=0 . \tag{2}$$

In these expressions, k is the wave vector, $\mathcal{P}$ is a real matrix element related to the momentum matrix element between conduction and valence states at the zone center, and $\varepsilon'=\varepsilon-(\hbar^2k^2/2m_0)$ where ε is the electron energy and m_0 the free-electron mass.

At large wave-vector limit, the asymptotic behavior of the Γ_6, Γ_{8l}, and Γ_7 bands can be deduced from Eq. (2):[3]

$$\begin{aligned}\varepsilon'_6&=[(E_G-\Delta/3)/2]+k\mathcal{P} ,\\ \varepsilon'_7&=[(E_G-\Delta/3)/2]-k\mathcal{P} ,\\ \varepsilon'_{8l}&=-2\Delta/3 .\end{aligned} \tag{3}$$

For small k values, the solutions of Eqs. (1) and (2) describe four parabolic bands. They yield the expressions of the effective masses m_6, m_{8h}, m_{8l}, m_7 (respectively, of the Γ_6, Γ_{8h}, Γ_{8l}, and Γ_7 bands) when the remote-band interaction is not taken into account (m_6 is defined as an electron mass and m_{8h}, m_{8l}, m_7 are defined as hole masses):

$$\begin{aligned}m_0/m_6&=1+P^2(E_G+2\Delta/3)/E_G(E_G+\Delta) ,\\ m_0/m_{8h}&=-1 ,\\ m_0/m_{8l}&=-[1-(2P^2/3E_G)] ,\\ m_0/m_7&=-\{1-[P^2/3(E_G+\Delta)]\} ,\end{aligned} \tag{4}$$

where $P^2=(2m_0/\hbar^2)\,\mathcal{P}^2$. The values of m_6, m_{8l}, and m_7 are not very different from the measured effective masses. In contrast, the experimental heavy-hole mass is determined by the remote-band interaction.

The expressions of the wave functions can be simply written in the basis chosen by Kane using the real coefficients a_i, b_i and c_i defined by

$$\begin{aligned}a_i&=k\mathcal{P}(\varepsilon'_i+2\Delta/3)/N_i ,\\ b_i&=\sqrt{2}(\Delta/3)(\varepsilon'_i-E_G)/N_i ,\\ c_i&=(\varepsilon'_i-E_G)(\varepsilon'_i+2\Delta/3)/N_i ,\end{aligned} \tag{5}$$

where the index i refers to the bands Γ_6, Γ_{8l}, and Γ_7, ε'_i is the relevant root of Eq. (2), and N_i is a normalizing factor defined by $a_i^2+b_i^2+c_i^2=1$.

Then the remote-band interaction is added as a perturbation through the matrix elements $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}$, $\mathcal{D}$, $\mathcal{F}$, $\mathcal{G}$

defined in Ref. 1, which can be estimated from the experimental values of the effective masses, the band-gap energy, the spin-orbit splitting energy, and the momentum matrix element P. For instance, along the [100] direction of the Brillouin zone we have

$$\begin{aligned} &m_0/m_6=m_0/m_6+F\ , \\ &(m_0/m_{8h})=(m_0/m_{8h})-(C+D)\ , \\ &(m_0/m_{8l})=(m_0/m_{8l})-[(C+D)/3]-[2(A+B)/3]\ , \\ &(m_0/m_7)=(m_0/m_7)-[2(C+D)/3]-[(A+B)/3]\ , \end{aligned} \tag{6}$$

where m_6, m_{8h}, m_{8l}, and m_7 are the experimental values of effective masses and A, B, C, D, F are related to $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}$, $\mathcal{D}$, $\mathcal{F}$ through formulas of the type $A=(2m_0/\hbar^2)\mathcal{A}$. The energy corrections involve these matrix elements as well as the coefficients a_i^2, b_i^2, and c_i^2.

III. SIMPLE ANALYTICAL DESCRIPTIONS OF THE CONDUCTION AND VALENCE BANDS

A. Principle

Our method consists in reducing Eq. (2) to a quadratic equation (i.e., in removing the coupling between one of the bands and the two others) and is based on the following considerations.

We start from a general cubic equation in the form

$$\begin{aligned} P(x)&=(x-a)(x-b)(x-c) \\ &=x^3-\Sigma x^2+\sigma x-\Pi=0\ . \end{aligned} \tag{7}$$

We take an arbitrary constant a and form the cubic equation which has the roots α, β, and γ such as $\alpha+\beta+\gamma=\Sigma$ and $\alpha\beta\gamma=\Pi$. We obtain

$$\wp(x)=x^3-\Sigma x^2+[\sigma-P(a)/a]x-\Pi=0\ . \tag{8}$$

We now choose α as a root of the equation $P(x)+f(x)=0$, where $f(x)$ is an arbitrary function. Then α is a root of the equation

$$\wp(x)=x^3-\Sigma x^2+[\sigma+f(a)/a]x-\Pi=0\ . \tag{9}$$

We now assume that $f(a)/a$ is small enough so that $\alpha=a+\delta a$, $\beta=b+\delta b$, and $\gamma=c+\delta c$, where δa, δb, and δc are small compared to a, b, and c, respectively. Because the sum and the product of the roots of Eqs. (7) and (9) are identical, this implies

$$\delta a+\delta b+\delta c=0\ , \tag{10}$$

and to first order

$$\delta a/a+\delta b/b+\delta c/c=0\ . \tag{11}$$

From the comparison of the coefficients of the linear terms in Eqs. (7) and (8) we also deduce

$$(b+c)\delta a+(a+c)\delta b+(a+b)\delta c=f(a)/a\ . \tag{12}$$

Then, from Eqs. (9)–(11), we get, for instance,

$$\delta a/a=-f(a)/[a(a-b)(a-c)]\ . \tag{13}$$

Consequently, α is a good approximation of the root a of Eq. (7) if $f(\alpha)/\alpha$ is small with respect to the product of the separations between a and the two other roots of Eq. (7). Also, the accuracy of different approximations of the roots can be compared simply through the functions $f(x)$ they are associated with. To estimate the error numerically, it can be convenient to make use of the relation

$$(a-b)(a-c)=3a^2-2\Sigma a+\sigma=[dP(x)/dx]_a \tag{14}$$

and to note that

$$\begin{aligned} [dP(x)/dx]_\alpha&=(3a^2-2\Sigma a+\sigma) \\ &\times\{1-(2\delta a/a)[a/(a-b)+a/(a-c)]\}\ . \end{aligned} \tag{15}$$

Thus, at the lowest order

$$\delta a/a\approx -f(\alpha)/\alpha[dP(x)/dx]_\alpha\ . \tag{16}$$

B. Analytical band expressions for $\Delta\leq E_G$

1. Precise band approximations

We now come back to the Kane model and remark that Eq. (2) can be written

$$\begin{aligned} P(\varepsilon')&=(\varepsilon'+2\Delta/3)[(\varepsilon'-E_G)(\varepsilon+\Delta/3)-(k\mathcal{P})^2] \\ &-(2\Delta^2/9)(\varepsilon'-E_G)=0 \end{aligned} \tag{17}$$

when using the relation

$$(\varepsilon'+2\Delta/3)(\varepsilon'+\Delta/3)-2\Delta^2/9=\varepsilon'(\varepsilon'+\Delta)\ .$$

We form the equation $P(\varepsilon')+f(\varepsilon')=0$ where $f(\varepsilon')=(2\Delta^2/9)(\varepsilon'-E_G)$ and obtain the two equations

$$\varepsilon'+2\Delta/3=0\ , \tag{18}$$

$$\varepsilon'^2-\varepsilon'(E_G-\Delta/3)-E_G\Delta/3-(k\mathcal{P})^2=0\ , \tag{19}$$

which yield

$$\begin{aligned} &\varepsilon'_6=[(E_G-\Delta/3)/2]+\mathcal{E}_1\ , \\ &\varepsilon'_7=[(E_G-\Delta/3)/2]-\mathcal{E}_1\ , \\ &\varepsilon'_{8l}=-2\Delta/3\ , \end{aligned} \tag{20}$$

where

$$\mathcal{E}_1=\{(k\mathcal{P})^2+[(E_G+\Delta/3)/2]^2\}^{1/2}\ .$$

These expressions describe mirror Γ_6 and Γ_7 bands, as Eqs. (3) already did. This simply expresses a two-band coupling between the Γ_6 and Γ_7 bands which quickly becomes dominant away from the zone center. It is readily verified from Eq. (13) that the approximation is extremely accurate for the conduction band when $\Delta\leq E_G$.[10] At the zone center, the conduction effective mass deduced from Eqs. (20) only differs from the effective mass deduced from the Kane expansion at small k [see Eqs. (4)] by the factor $1-2\Delta^2/9E_G^2$ (at second order) and, whatever the ratio Δ/E_G, the correct asymptotic behavior given by Eqs. (3) is predicted for the three bands. For the Γ_{8l} and

Γ_7 bands the approximation only holds when $E_G\Delta/(k\mathcal{P})^2$ is notably smaller than unity. In Figs. 1–3, the errors on the Γ_6, Γ_7, and Γ_{8l} bands are plotted for different Δ/E_G ratios. They have been estimated from Eq. (13).

We choose the precise Γ_6 band approximation given by Eqs. (20) and form the related $\wp(\varepsilon')$. According to Eq. (9), we deduce the quadratic equation which determines approximations of the Γ_{8l} and Γ_7 band dispersions:

$$\varepsilon'^2+\varepsilon'[\mathcal{E}_1-(E_G-5\Delta/3)/2]+(2\Delta/3)(k\mathcal{P})^2 \times[\mathcal{E}_1+(E_G-\Delta/3)/2]^{-1}=0 . \quad (21)$$

Equation (21) provides very accurate but somewhat more complicated expressions of ε'_{8l} and ε'_7:

$$\varepsilon'_7=-(\varepsilon'_6-E_G+\Delta)/2-\mathcal{E}_2 , \quad (22)$$

$$\varepsilon'_{8l}=-(\varepsilon'_6-E_G+\Delta)/2+\mathcal{E}_2 , \quad (23)$$

where

$$\mathcal{E}_2=\{[(\varepsilon_6'-E_G+\Delta)/2]^2 -[(2\Delta/3)(\varepsilon'_6-E_G)(\varepsilon'_6+\Delta/3)/\varepsilon'_6]\}^{1/2} ;$$

here we have made use of the relation $(k\mathcal{P})^2=(\varepsilon'_6-E_G)(\varepsilon'_6+\Delta/3)$.

The approximate solutions of Eq. (2), ε'_6 given by Eqs. (20), ε_7' and ε_{8l}' given by Eqs. (22) and (23), are the solutions of $P(\varepsilon')+f(\varepsilon')=0$, where $f(\varepsilon')=\varepsilon'(2\Delta^2/9)(\varepsilon'_6-E_G)/\varepsilon'_6$; here we remark that

$$(\varepsilon'_6-E_G)/\varepsilon'_6=[\mathcal{E}_1-(E_G+\Delta/3)/2] \times[\mathcal{E}_1+(E_G-\Delta/3)/2]^{-1} .$$

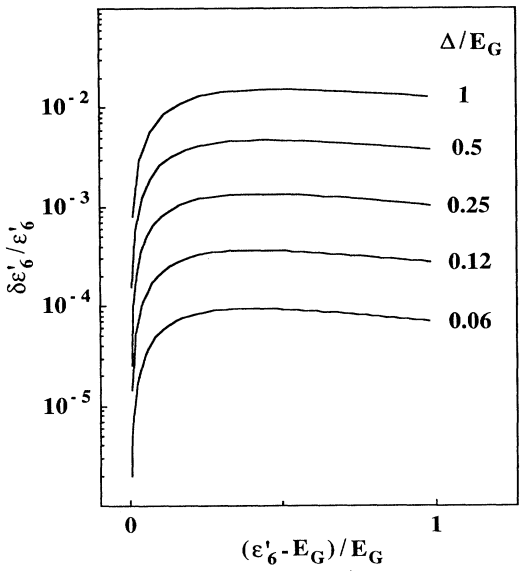

FIG. 1. Relative error on the approximate electron energy in the Γ_6 band given by Eqs. (20). The error has been estimated using Eq. (14), starting from Eq. (2) with $f(\varepsilon')=(2\Delta^2/9)(\varepsilon'-E_G)$. The set of curves is drawn as a function of the electron *kinetic* energy normalized to the band-gap energy, for different values of the ratio Δ/E_G.

Using Eq. (13), the relative errors on the dispersions of the Γ_7 and Γ_{8l} bands can be straightforwardly estimated. They are plotted in Figs. 2 and 3, respectively.

2. *Simpler expressions of the valence bands*

To obtain a simple description of the Γ_{8l} band, we need simple expressions of the Γ_6 and Γ_7 bands which are equivalent to $\pm k\mathcal{P}$ *at large* k and have the correct limits *at* $k=0$. The first condition provides the *correct limit at large* k of the Γ_{8l} band and the second ensures the *correct effective mass* and *limit at the zone center* of the light-hole band because roots of Eq. (2) are related through the equation

$$\varepsilon'_6\varepsilon'_7\varepsilon'_{8l}=(2\Delta/3)(k\mathcal{P})^2 . \quad (24)$$

We obtain the following convenient expressions:

$$\varepsilon'_6=[(E_G-\Delta)/2]+\mathcal{E}_3 , \quad (25)$$

$$\varepsilon'_7=[(E_G-\Delta)/2]-\mathcal{E}_3 , \quad (26)$$

where

$$\mathcal{E}_3=\{(k\mathcal{P})^2+[(E_G+\Delta)/2]^2\}^{1/2} ,$$

by choosing $f(\varepsilon')=(2\Delta/3)(k\mathcal{P})^2$. Then using Eqs. (24)–(26), we get

$$\varepsilon'_{8l}=-(2\Delta/3)/[1+E_G\Delta/(k\mathcal{P})^2] . \quad (27)$$

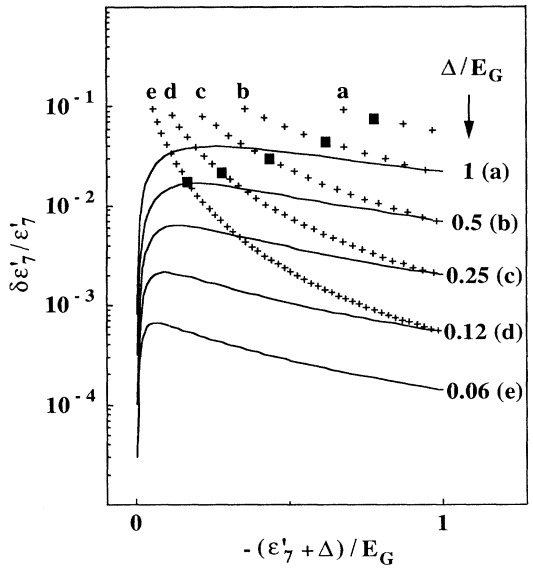

FIG. 2. Relative error on the approximations of the electron energy in the Γ_7 band given by Eqs. (20) (crosses), and Eq. (23) (solid lines). The errors have been estimated using Eq. (14), starting from Eq. (2) with $f(\varepsilon')=(2\Delta^2/9)(\varepsilon'-E_G)$ in the case of the first approximation [Eqs. (20); ■ indicates qualitatively the domain of validity of this approximation as it corresponds to $E_G\Delta/(k\mathcal{P})^2=\frac{1}{4}$] and $f(\varepsilon')=\varepsilon'(2\Delta^2/9)(\varepsilon'_6-E_G)/\varepsilon_6'$ in the case of the second approximation [Eq. (23)]. The sets of curves are drawn as a function of the electron *kinetic* energy normalized to the band-gap energy, for different values (*a*, *b*, *c*, *d*, and *e*) of the ratio Δ/E_G.

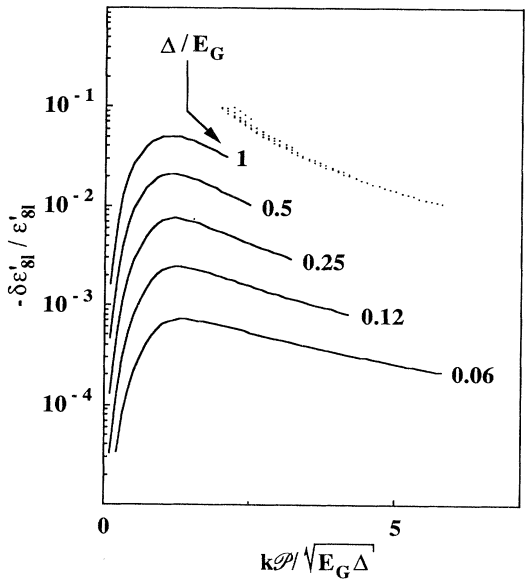

FIG. 3. Relative error on the approximations of electron energy in the Γ_{8l} band given by Eqs. (20) (dotted lines), and Eq. (22) (solid lines). The errors have been estimated using Eq. (14), starting from Eq. (2) with $f(\varepsilon')=(2\Delta^2/9)(\varepsilon'-E_G)$ in the case of the first approximation [Eqs. (20)], and $f(\varepsilon')=\varepsilon'(2\Delta^2/9)(\varepsilon'_6-E_G)/\varepsilon'_6$ in the case of the second approximation [Eq. (23)]. The sets of curves are drawn as a function of the electron *kinetic* energy normalized to the band-gap energy, for different values of the ratio Δ/E_G. In each case, the calculation has been performed until $(\varepsilon'_7+\Delta)/E_G=-1$. The error on the approximation given by Eq. (20) is small only at large k and little sensitive to the ratio Δ/E_G.

Equation (27) provides a correct qualitative description of the Γ_{8l} band. For instance, in the case of InP, this expression is accurate within a maximum error of about 10 meV.

From Eqs. (25) and (27), and because $\varepsilon'_6+\varepsilon'_{8l}+\varepsilon'_7=E_G-\Delta$, we can also deduce a simple and accurate expression of ε'_7:

$$\varepsilon'_7=[(E_G-\Delta)/2]-\mathcal{E}_3+\{(2\Delta/3)[1+E_G\Delta/(k\mathcal{P})^2]\} . \tag{28}$$

This expression has the right limit in $k=0$, the correct asymptotic behavior, and yields a split-off effective mass which differs from Kane's [given by Eqs. (4)] by a factor $1-2\Delta/E_G$.

A simple approximation of ε'_7 giving the right spin-orbit effective mass can be, of course, obtained by applying the method that we describe in Sec. III A. Taking the origin of energy *at the top of the spin-orbit split band* and choosing $f(\varepsilon')=-2\varepsilon'^2(E_G+2\Delta/3)$, the solutions of Eq. (9) are given by

$$\begin{aligned}&\varepsilon'_7=m'_7P^2/2m_0-\mathcal{E}_4 ,\\ &\varepsilon'^2-\varepsilon'(E_G+2\Delta-\varepsilon'_7)-(\Delta/3\varepsilon'_7)(k\mathcal{P})^2=0 ,\end{aligned} \tag{29}$$

where $m'_7/m_0=3(E_G+\Delta)/P^2$ is the Γ_7 band effective mass calculated in the Kane model when the remote-band interaction is not added and neglecting the free-electron contribution [see Eqs. (4)] and $\mathcal{E}_4=[(k\mathcal{P})^2+(m'_7P^2/2m_0)^2]^{1/2}$. The expression of ε'_7 given by Eqs. (29) is accurate around $k=0$ but becomes very quickly a poor approximation away from the zone center, as indicated by the rapid divergence of $f(\varepsilon')$.

It is not surprising that a somewhat more complicated expression is needed to describe precisely the Γ_7 band dispersion because the Γ_7 is mainly coupled to the Γ_{8l} band near the zone center and to the Γ_6 band away from the zone center. These two "coupling regimes" are, for instance, revealed in Eq. (28).

C. The remote-band interaction and the wave functions

The procedure followed in the Kane model, to calculate the expressions of the wave functions and the interaction with the remote bands, is recalled in Sec. II. For both calculations, only the expressions of the Kane coefficients a_i^2, b_i^2, and c_i^2 remain to be determined.

For the Γ_6 and Γ_7 bands, we start from the approximate solutions of the secular equation given by Eqs. (20) and we make use of the relation

$$(k\mathcal{P})^2=[\mathcal{E}_1-(E_G+\Delta/3)/2][\mathcal{E}_1+(E_G+\Delta/3)/2] . \tag{30}$$

We straightforwardly obtain the very simple expressions of the Kane coefficients:

$$\begin{aligned}&a_j^2=A_j^2/(1+B_j^2) ,\\ &b_j^2=B_j^2/(1+B_j^2) ,\\ &c_j^2=C_j^2/(1+B_j^2) ,\end{aligned} \tag{31}$$

where

$$\begin{aligned}&A_j^2=\tfrac{1}{2}(\varepsilon'_j+\Delta/3)/[\varepsilon'_j-(E_G-\Delta/3)/2] ,\\ &C_j^2=\tfrac{1}{2}(\varepsilon'_j-E_G)/[\varepsilon'_j-(E_G-\Delta/3)/2] ,\\ &B_j^2=[(2\Delta^2/9)/(\varepsilon'_j+2\Delta/3)^2]C_j^2 .\end{aligned} \tag{32}$$

In the above expressions the index j refers to the Γ_6 or Γ_7 bands. Note that the coefficients A_j^2, B_j^2, and C_j^2 can also be written

$$\begin{aligned}&A_6^2=C_7^2=\tfrac{1}{2}[1+(E_G+\Delta/3)/2\mathcal{E}_1] ,\\ &C_6^2=A_7^2=\tfrac{1}{2}[1-(E_G+\Delta/3)/2\mathcal{E}_1] ,\\ &B_6^2=\{(2\Delta^2/9)/[\mathcal{E}_1+(E_G+\Delta)/2]^2\}C_6^2 ,\\ &B_7^2=\{(2\Delta^2/9)/[\mathcal{E}_1-(E_G+\Delta)/2]^2\}C_7^2 .\end{aligned} \tag{33}$$

For the Γ_{8l} band, when we use the asymptotic description given by Eqs. (20), we simply have $a_{8l}^2=c_{8l}^2=0$, $b_{8l}^2=1$. Taking the better approximation of ε'_{8l} given by Eq. (27), we obtain more general and accurate expressions of the Kane coefficients:

$$\begin{aligned}&a_{8l}^2=A_{8l}^2/(1+A_{8l}^2) ,\\ &b_{8l}^2=B_{8l}^2/(1+A_{8l}^2) ,\\ &c_{8l}^2=C_{8l}^2/(1+A_{8l}^2) ,\end{aligned} \tag{34}$$

where

$$A_{8l}^2=(2\Delta/E_G)[(u-1)/(u^2+2)] \times\{[1+(2\Delta/3E_G)(u-1)/u]^2\}^{-1},$$
$$B_{8l}^2=u^2/(u^2+2), \quad (35)$$
$$C_{8l}^2=2/(u^2+2),$$

with

$$u=1+(k\mathcal{P})^2/E_G\Delta .$$

When Δ is not too large compared to E_G, it is readily checked that B_6^2 and B_7^2 can be neglected with respect to unity in the expressions of a_6^2, b_6^2, c_6^2, a_7^2, b_7^2, and c_7^2. In other respects, A_{8l}^2 is small compared to 1 in the k range where the model holds, and can also be neglected in the expression of a_{8l}^2, b_{8l}^2, and c_{8l}^2. Therefore, A_i^2, B_i^2, and C_i^2 are generally very good approximations of the coefficients a_i^2, b_i^2, and c_i^2. They can also be used to write simple expressions of the eigenfunctions and of the remote-band interaction.

We remark that we have also obtained $a_6\approx c_7$ and $a_7\approx -c_6$. This again results from the two-band coupling between the Γ_6 and Γ_7 bands through the real matrix element $k\mathcal{P}$. Analogously, *at the zone center,* $b_7=c_{8l}$ and $b_{8l}=-c_7$ because of the two-band coupling between the Γ_{8l} and Γ_7 bands.

IV. OTHER APPROACHES

A. Rode's empirical model for conduction band

To study low-field transport in semiconductors, Rode uses an analytical expression of the Γ_6 band dispersion deduced from a two-band model.[4] He treats the case where $\Delta=0$, and remarks that the approximation remains satisfactory even for large Δ [when $\Delta=0$, the expression of ε_6' given by Eqs. (20) is equivalent to Rode's formula, Eq. (4) of Ref. 4, when the free-electron contribution is not added]. Then, he fits empirically $\mathcal{P}$ to the experimental conduction effective mass: this way the remote-band interaction is somehow taken into account. Fawcett and Ruch propose a similar model but add in the expression of the Γ_6 band dispersion a factor which takes into account nonparabolicity higher-order effects:[5] the expansion around $k=0$ of their formula is then equivalent to the expansion at fourth order of Kane's solution. More recently, Rode's approach has been used by Johnson *et al.* in a slightly different way.[9] These authors first introduce the conduction effective mass deduced from the second-order expansion at small k of Kane's solution calculated when the remote-band interaction and the free-electron contribution are not added (this is equivalent to Rode's model but in the more general case where $\Delta\neq 0$). Then, following Rode's procedure, they introduce the experimental effective mass through a fit of $\mathcal{P}$. In fact, these approximate solutions of Kane's model for the conduction band can be simply obtained and studied from the method described in Sec. II.

We rewrite Eq. (2) with the origin of energy *at the bottom of the conduction band* and solve the equation $P(\varepsilon')+f(\varepsilon')=0$, where $f(\varepsilon')=-\varepsilon'^2(2\Delta^2/9)/(E_G+2\Delta/3)$. We obtain

$$\varepsilon'+E_G+2\Delta/3=0 . \quad (36)$$
$$\varepsilon'^2-\varepsilon' E_G(E_G+\Delta)/(E_G+2\Delta/3)-(k\mathcal{P})^2=0 , \quad (37)$$

which yield

$$\varepsilon_6'=-m_6'P^2/2m_0+\mathcal{E}_5 ,$$
$$\varepsilon_7'=-m_6'P^2/2m_0-\mathcal{E}_5 , \quad (38)$$
$$\varepsilon_{8l}'=-E_G-2\Delta/3 ,$$

where

$$\mathcal{E}_5=[(k\mathcal{P})^2+(m_6'P^2/2m_0)^2]^{1/2}$$

and

$$m_6'/m_0=E_G(E_G+\Delta)/(E_G+2\Delta/3)P^2$$

is the conduction effective mass calculated in the Kane model when the remote-band interaction is not added and neglecting the free-electron contribution [see Eqs. (4)]. The expression of ε_6' given by Eqs. (38) corresponds to Rode's formula [Eq. (4) of Ref. 4] when $\Delta\neq 0$ and the free-electron contribution is not added. *Close to the zone center,* this approximation is somewhat more precise than the one given by Eqs. (20) and still holds at large Δ/E_G ratios (the result of Fawcett and Ruch is even better as it fits to the Kane expansion at fourth order but is more complicated). Nevertheless, the improvement of the Γ_6 band description is not significant when $\Delta\leq E_G$ because the errors plotted in Fig. 1 are very small. *At large k,* Rode's approximation does not yield the exact asymptotic behavior and is therefore not as good as Eqs. (20) [the asymptotic line being upshifted by $\Delta^2/g(E_G+2\Delta/3)$].

With the above approximation, the remote-band interaction can be easily calculated just as in Sec. III C [Eqs. (38) are very similar to Eqs. (20)]. The added terms involve the matrix element $\mathcal{I}$ which enters the experimental conduction effective mass [see Eqs. (6)] but also other matrix elements like $\mathcal{A}$ and $\mathcal{B}$. In contrast, as Eqs. (38) exhibit the conduction effective mass deduced from the three-band model, Rode and other authors[4,5,9] introduce the remote-band interaction by fitting empirically P to the *experimental* conduction effective mass. With respect to Kane's theory, this procedure only involves the matrix element $\mathcal{I}$. The remote-band interaction is therefore not properly taken into account.

B. The D'yakonov-Perel' model for the valence bands

To perform spin-polarization analysis, D'yakonov and Perel' have calculated analytical approximations of the Γ_{8l} and Γ_7 bands.[6] They start from Luttinger's Hamiltonian[11] and use symmetry considerations. Their treatment leaves an uncoupled parabolic Γ_6 band. They obtain precise descriptions of the valence bands when the kinetic energy and Δ are small compared to E_G. Using the Kane expressions of the effective masses when the remote-band interaction and the free-electron contribu-

tion are not added, their result can be written

$$\varepsilon_7' = -[(k\mathcal{P})^2 + E_G\Delta]/2E_G - (\{[(k\mathcal{P})^2 + E_G\Delta]/2E_G\}^2 - (2\Delta/3E_G)(k\mathcal{P})^2)^{1/2} , \quad (39)$$

$$\varepsilon_{8l}' = -[(k\mathcal{P})^2 + E_G\Delta]/2E_G + (\{[(k\mathcal{P})^2 + E_G\Delta]/2E_G\}^2 - (2\Delta/3E_G)(k\mathcal{P})^2)^{1/2} . \quad (40)$$

In fact, this formulation can also be deduced from Kane's theory, following the method described in Sec. II and choosing

$$f(\varepsilon') = -(k\mathcal{P})^2[(k\mathcal{P}/E_G)^2(\varepsilon' + 2\Delta/3) - \varepsilon'(\Delta/3E_G)] .$$

Then, a parabolic conduction band is factorized and the solutions of the resulting quadratic equation are exactly Eqs. (39) and (40). An alternative way consists in calculating the second-order expansion at small k of the Γ_6 band approximation given by Eqs. (20). We obtain

$$\varepsilon_6' = E_G + (k\mathcal{P})^2/(E_G + \Delta/3) . \quad (41)$$

Carrying this expression into Eqs. (22) and (23) we obtain again Eqs. (39) and (40).

The function $f(\varepsilon')$ shows that this result is only precise in the low-kinetic-energy range, as mentioned by D'yakonov and Perel'. In particular, the Γ_{8l} band approximation is accurate in a wide k range while the Γ_7 band approximation only holds around $k=0$. This is evidenced by Eq. (39) which describes a parabolic Γ_7 band away from the zone center and results again from the two-band coupling between the Γ_7 band and the Γ_6 band which is parabolic in the present case.

V. CONCLUSION

We have described in this paper a general method to derive analytical approximations of the solutions of the Kane band model and to estimate their accuracy. Various algebraic band descriptions used in the past[3–6,9] have been deduced here from Kane's theory in the framework of our procedure. This analysis brings out a clear insight into these previous models. Moreover, we have obtained approximations of the Kane solutions for the conduction and valence bands which include the remote-band interaction and are extremely accurate. The description of the conduction band is particularly simple. This is interesting as it should make easier transport calculations throughout a wide energy range. We have also derived expressions of the eigenfunctions which are very convenient and, therefore, useful for many applications as, for instance, the interpretation of experiments involving electron-spin properties: the spin splitting of the conduction band, which acts as a spin-precession vector,[1,3,6,7] is directly related to the product $a_6 b_6$ and therefore can be expressed in a form well suited for subsequent calculation. Finally, these approximations of the dispersion of the conduction and valence bands can be successfully used to analyze band-structure measurements and to determine their sensitivity to various parameters.[12]

ACKNOWLEDGMENTS

We are indebted to G. Lampel for his constant interest and for many stimulating discussions. We thank C. Hermann, G. Lampel, and D. Paget for a critical reading of the manuscript. H.-J.D. is a member of the Direction des Recherches, Etudes et Techniques de la Délégation Générale pour l'Armement. Laboratoire de Physique de la Matière Condensée is "Unité de Recherche Associée D-1254 au Centre National de la Recherche Scientifique."

[1] E. O. Kane, J. Phys. Chem. Solid **1**, 249 (1957).
[2] J. S. Blakemore, J. Appl. Phys. **53**, R123 (1982).
[3] H. Riechert, H.-J. Drouhin, and C. Hermann, Phys. Rev. B **38**, 4136 (1988).
[4] D. L. Rode, in *Semiconductors and Semimetals,* edited by R.K. Willardson and A. C. Beer (Academic, New York, 1975), Vol. 10, p. 1.
[5] W. Fawcett and J. G. Ruch, Appl. Phys. Lett. **15**, 368 (1969).
[6] M. I. D'yakonov and V. I. Perel', Zh. Eksp. Teor. Fiz. **60**, 1954 (1971) [Sov. Phys. JETP **33**, 1053 (1971)].
[7] G. Fishman and G. Lampel, Phys. Rev. B **16**, 820 (1977).
[8] B. P. Zakharchenya, D. N. Mirlin, V. I. Perel', and I. I. Reshina, Usp. Fiz. Nauk. **136**, 459 (1982) [Sov. Phys. Usp. **25**, 143 (1982)].
[9] E. A. Johnson, A. MacKinnon, E. P. O'Reilly, and M. Silver, Phys. Rev. Lett. **65**, 752 (1990).
[10] The expression given by Eqs. (20) for the conduction band is similar to the formula used by T. Ruf and M. Cardona [Phys. Rev. B **41**, 10 747 (1990)] in the absence of remote band interaction.
[11] J. M. Luttinger, Phys. Rev. **102**, 1030 (1956).
[12] J. Peretti, H.-J. Drouhin, D. Paget, and A. Mircéa, following paper, Phys. Rev. B **44**, 7990 (1991).