Analytic dispersion relations near the Γ point in strained zinc-blende crystals

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(Received 28 May 1991)

An eight-band $\mathbf{k}\cdot\mathbf{p}$ model of the electronic states near the Γ point of a strained zinc-blende semiconductor is renormalized using Löwdin perturbation theory. The renormalization leads to matrices of reduced dimensionality, 2×2, 4×4, and 2×2, for the conduction, light- and heavy-hole, and spin-orbit split-off bands, respectively. The reduced dimensionality of these matrices allows us to obtain analytic dispersion relations in the presence of small but arbitrary strains. Comparison of the analytic dispersion relations is made to those obtained by numerically diagonalizing the eight-band model for the case of biaxially strained and unstrained GaAs.

I. INTRODUCTION

Energy bands in strained semiconductors, such as Si and Ge, have been the subject of several theoretical investigations.[1–4] More recently, the direct-gap semiconductors with zinc-blende structure, such as GaAs and GaP, are attracting considerable attention because of their applications in the area of optoelectronic devices.[5–9] Energy bands in strained semiconductors are frequently treated by $\mathbf{k}\cdot\mathbf{p}$-type models, leading to matrices whose dimensionality depends on the small point group of $\mathbf{k}$ (the appropriate symmetry group at the critical point in the Brillouin zone) and the number of bands that are included in the model.[10] For example, near the Γ point in the Brillouin zone of a direct-gap zinc-blende semiconductor, the band structure in the vicinity of the fundamental gap is accurately described by an eight-band $\mathbf{k}\cdot\mathbf{p}$ model, whose basis states form basis functions for the T_d double group.[11,12] This formulation includes effects resulting from the lack of inversion symmetry but leads to 8×8 matrices which must be diagonalized numerically.

In this work we formulate a renormalization procedure based on Löwdin perturbation theory[13] which allows one to derive analytic dispersion relations in terms of the parameters in the original model. As a concrete example we demonstrate this renormalization procedure using an eight-band $\mathbf{k}\cdot\mathbf{p}$ model[9] of the energy bands near the Γ point of strained zinc-blende crystals. The model includes the conduction band, the (light- and heavy-hole) valence bands, and spin-orbit split-off bands. Löwdin perturbation theory is used to derive the 8×8 renormalized interaction matrix, $U=H+D$, which describes the band structure near the Γ point. The matrix H is essentially the eight-band Kane model[11] and is independent of strain, and D contains the strain interactions to first order.[9] We use Löwdin perturbation theory to perform a second renormalization on the matrix U, leading to matrices of smaller dimensions, 2×2, 4×4, and 2×2, for the conduction, light- and heavy-hole, and spin-orbit bands, respectively. These second-renormalized matrices describe the band structure near the Γ point and are functions of the material parameters that appear in the original eight-band model. The reduced dimensionality of these matrices allows us to obtain analytic results for electron dispersion relations near $\mathbf{k}=0$, in the presence of arbitrary strain. In what follows, we calculate these second-renormalized matrices and the resulting dispersion relations for the conduction, light- and heavy-hole, and spin-orbit bands. We then compare the accuracy of the analytic results with that obtained by numerically diagonalizing the eight-band model for the case of a specific material system.

II. SECOND RENORMALIZATION

In the strained eight-band model the conduction-band states at $\mathbf{k}=\mathbf{0}$ form a basis for the Γ_6 irreducible representation of the T_d double group.[14] The states at $\mathbf{k}=\mathbf{0}$ for the light and heavy holes, and for the spin-orbit split-off states, form a basis for the Γ_8 and Γ_7 irreducible representations, respectively. See Ref. 9 for definitions of these basis states. In this basis, the total Hamiltonian matrix of the eight-band model is given by $U=H+D$, where H is essentially the eight-band Kane model (independent of strain) and D is the strain interaction matrix whose elements are linear in strain. The 8×8 matrices H and D are given in Eqs. (A1) and (A6), respectively. The matrix H depends on the modified Luttinger parameters, γ_1, γ_2, and γ_3 [which are functions of the Luttinger parameters[15] γ_1^L, γ_2^L, and γ_3^L; see Eq. (A3)], the valence-band–conduction-band mixing parameter P_0, the mixing with higher bands A', and the energy gaps at $\mathbf{k}=\mathbf{0}$ (between the conduction and valence band, $E_g=E_c-E_v$, and between the valence and spin-orbit band, Δ). The strain interaction matrix D depends on the deformation-potential constants a', b', a, b, and d. The deformation-potential constants a' and b' describe the coupling of the conduction band to strain and a, b, and d are the Pikus and Bir[1,2,5] deformation-potential constants describing the coupling of the valence band to strain. See Ref. 9 for precise definitions of these deformation-potential constants.

We now perform a second Löwdin renormalization on the matrix U. For the conduction band, we treat the Γ_6

conduction-band states as class-A states and the Γ_8 and Γ_7 basis states as class-B states.[13] The second-renormalized conduction-band matrix $U_{cc'}^{\rm cond}$ can then be written as a sum of two 2×2 matrices,

$$U_{cc'}^{\rm cond}=U_{cc'}^{(0)}+U_{cc'}^{(1)}\ , \tag{1}$$

where $U_{cc'}^{(0)}$ describes the conduction band in the absence of strain and $U_{cc'}^{(1)}$ describes the renormalized strain interactions, with matrix elements linear in strain components. Third-order Löwdin renormalization leads to

$$U_{cc'}^{(0)}=H_{cc'}+\sum_n^B \frac{H_{cn}H_{nc'}}{\bar{E}-H_{nn}}+\sum_n^B\sum_{n'}^B \frac{H_{cn}H_{nn'}H_{n'c'}}{(\bar{E}-H_{nn})(\bar{E}-H_{n'n'})}\ , \tag{2}$$

where the elements of $U_{cc'}^{(0)}$ are correct to fourth order in wave vector.[16] The indices c and n refer to class-A and -B states, respectively. Matrix elements $H_{cc'}$ and $H_{nn'}$ are second order in wave vector, while matrix elements that connect class-A and -B states, H_{nc}, are linear in wave vector. The second-renormalized strain interaction matrix is given by

$$U_{cc'}^{(1)}=D_{cc'}+\sum_n^B\left[\frac{H_{cn}H_{nc'}}{\bar{E}-H_{nn}}\frac{D_{nn}}{\bar{E}-H_{nn}}+\frac{H_{cn}D_{nc'}+D_{cn}H_{nc'}}{\bar{E}-H_{nn}}\right], \tag{3}$$

where the elements of $U_{cc'}^{(1)}$ are correct to linear order in strain and quadratic order in wave vector. The first term in Eq. (3) represents the direct strain interactions among the Γ_6 states and the second term represents the renormalization of the effective mass due to the presence of strain. The above renormalization procedure is reasonable for wide-gap semiconductors such as GaAs since, for small wave vectors and small strain, the off-diagonal elements are small compared to the band gaps at[17] $\mathbf{k}=\mathbf{0}$, $|H_{cn}|\ll|H_{cc}-H_{nn}|$. We linearize the eigenvalue problem for the conduction band by taking $\bar{E}=(H_{11}+H_{22})/2$. Since the wave vector $\mathbf{k}$ and strain e_{ij} are both small quantities, the matrix elements of $U_{cc'}^{\rm cond}$ are expanded in a power series in wave vector and strain components. The conduction-band dispersion relations are then found from the eigenvalues of the resulting 2×2 matrix. In order to carry out this renormalization procedure, a substantial amount of computation was required. A symbolic manipulation program known as MATHEMATICA was used for much of the computation.[18]

For the light- and heavy-hole valence bands the second-renormalized matrix is defined the same way as in Eqs. (1)–(3) except that the Γ_8 states are taken as class-A states and the Γ_6 and Γ_7 states are taken as class-B states. In this latter case we take $\bar{E}=(H_{33}+H_{44}+H_{55}+H_{66})/4$. The spin-orbit band is treated in an analogous fashion.

III. CONDUCTION BAND

The dispersion relations for the conduction bands are found from the eigenvalues of $U_{cc'}^{\rm cond}$ which can be written as

$$E_c=(E_c^{(0)}+E_c^{(1)})[1\pm(\delta\varepsilon_c^{(0)}+\delta\varepsilon_c^{(1)})^{1/2}]\ , \tag{4}$$

where the quantities $E_c^{(0)}$ and $\delta\varepsilon_c^{(0)}$ are independent of strain and $E_c^{(1)}$ and $\delta\varepsilon_c^{(1)}$ are linear in strain. These quantities are given by[19,20]

$$\begin{aligned}E_c^{(0)}=&E_g+\mathbf{k}^2\left[\tfrac{1}{2}+A'+P_0^2\frac{E_g+\frac{2}{3}\Delta}{E_g(E_g+\Delta)}\right]\\&-\tfrac{1}{3}(k_x^4+k_y^4+k_x^4)P_0^2\left\{\frac{1}{E_g^2}(1+2\gamma_2+\gamma_1+2A')+\frac{1}{2(E_g+\Delta)^2}\left[1+\gamma_1+2A'+8\gamma_2\left[1+\frac{\Delta}{E_g}\right]\right]\right\}\\&+(k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2)\left[\frac{2P_0^2}{3E_g^2}(\gamma_2-\gamma_1-3\gamma_3-2A'-1)+\frac{4P_0^2}{3E_g(E_g+\Delta)}(\gamma_2-3\gamma_3)\right.\\&\left.-\frac{P_0^2}{3(E_g+\Delta)^2}(\gamma_1+2A'+1)+B^2\frac{E_g+\frac{2}{3}\Delta}{E_g(E_g+\Delta)}\right],\end{aligned} \tag{5}$$

$$\begin{aligned}E_c^{(1)}=&a'\mathrm{tr}(\overleftrightarrow{e})-\tfrac{2}{3}P_0^2\mathbf{k}^2\mathrm{tr}(\overleftrightarrow{e})\left[\frac{a-b}{E_g^2}+\frac{3E_g+2(\Delta-b)}{E_g(E_g+\Delta)}+\frac{a}{2(E_g+\Delta)^2}\right]\\&-\frac{P_0^2}{3}[k_x^2(e_{yy}+e_{zz})+k_y^2(e_{zz}+e_{xx})+k_z^2(e_{xx}+e_{yy})]\left[\frac{2a+b}{E_g^2}+\frac{a}{(E_g+\Delta)^2}+\frac{2b}{E_g(E_g+\Delta)}\right]\\&+(k_xk_ye_{xy}+k_yk_ze_{yz}+k_xk_ze_{xz})\frac{2}{3E_g(E_g+\Delta)}\left[(b'B-2P_0^2)(3E_g+2\Delta)+\sqrt{3}dP_0^2\left[3+\frac{\Delta}{E_g}\right]\right],\end{aligned} \tag{6}$$

$$\delta\varepsilon_c^{(0)}=\frac{4}{9}\left[\frac{B\Delta P_0}{E_g^2(E_g+\Delta)}\right]^2[\mathbf{k}^2(k_x^2k_y^2+k_y^2k_z^2+k_x^2k_z^2)-9k_x^2k_y^2k_z^2]\ , \tag{7}$$

$$\delta\varepsilon_c^{(1)}=\tfrac{8}{9}Bb'P_0^2\left[\frac{\Delta}{E_g^2(E_g+\Delta)}\right]^2[e_{xy}k_xk_y(k_x^2+k_y^2)+e_{xz}k_xk_z(k_x^2+k_z^2)+e_{yz}k_yk_z(k_y^2+k_z^2)$$
$$-2k_xk_yk_z(e_{xy}k_z+e_{yz}k_x+e_{xz}k_y)]\ . \tag{8}$$

In Eq. (4) we have dropped second-order strain terms under the square root. The signs ± give the dispersion for each of the two conduction bands. The coefficient of $\mathbf{k}^2$ in $E_c^{(0)}$ gives the conduction-band effective mass in the absence of strain in terms of the material parameters in the eight-band model and agrees with the result given by Smith and Mailhiot.[21] The bare-electron mass is modified by terms proportional to P_0^2, due to direct mixing with valence bands, and is proportional to A' due to the coupling of the conduction band to higher bands outside the initial eight-dimensional manifold. Terms containing quartic powers of wave vector are band nonparabolicity terms resulting from band mixing with the valence band. This mixing is of two types, direct mixing of conduction and valence bands (the terms proportional to P_0^2) and mixing via intermediate states outside the original eight-dimensional manifold (the terms proportional to P_0^2A'). The term in $E_0^{(0)}$ containing $k_x^2k_y^2$ is a band warping term. Just as the light- and heavy-hole bands are warped, so are the conduction bands. However, here the conduction-band warping is not due to degeneracy, as is the case with the valence band. Instead, the warping results from mixing with the valence band (terms proportional to P_0) and also from the lack of inversion symmetry (terms proportional to B). If inversion symmetry were present, the terms proportional to B would be identically zero, i.e., $\delta\varepsilon_c^{(0)}=0$ and $\delta\varepsilon_c^{(1)}=0$, and consequently the conduction-band dispersion would be doubly degenerate and given by $E_c^{(0)}+E_c^{(1)}$. For the case of zero strain, Eq. (4) gives $2(\delta\varepsilon_c^{(0)})^{1/2}$ for the splitting of the conduction bands which is in agreement with the result obtained by Kane.[11] Note that to the order of this calculation, the bands are doubly degenerate along the k_x, k_y, and k_z directions. At finite strain, the cubic symmetry of the crystal is generally broken and the conduction-band dispersions are modified by a direct term proportional to $a'\mathrm{tr}(\overleftrightarrow{\varepsilon})$ and by terms proportional to P_0 which result from mixing with the valence band.

In order to ascertain the effect and accuracy of the renormalization procedure, we compare the GaAs conduction-band dispersion, obtained by numerical diagonalization of the eight-band model, with the analytic expression given in Eq. (4), for the cases of zero and finite biaxial strain.[22] Figure 1 shows a plot of the unstrained and strained conduction band calculated by numerically diagonalizing the eight-band model. We have introduced the convenient length $l_0=2.760$ Å, which renders $\hbar^2/m_0l_0^2=1$ eV. (The X point in the Brillouin zone is approximately at $k_xl_0=3.07$.) Figure 2 shows the comparison between the analytic dispersions in Eq. (4) and those obtained numerically from the eight-band model. The curve labeled H_{11} shows a plot of the (1,1) element of H (at zero strain) and represents the bare-electron dispersion. The curve labeled $H_{11}+D_{11}$ is a plot of the sum of the (1,1) elements of H and D and takes into account the energy shift due to the diagonal strain interaction. The numerically calculated dispersion relations from the

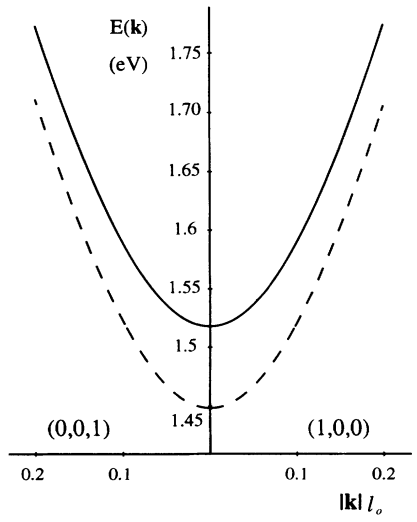

FIG. 1. The conduction band of GaAs, as calculated by numerically diagonalizing the eight-band model, is shown for the case of zero strain (solid line) and biaxial strain (dashed line) (see Table I), along the (1,0,0) and (0,0,1) $\mathbf{k}$-space directions. The convenient length $l_0=2.760$ Å.

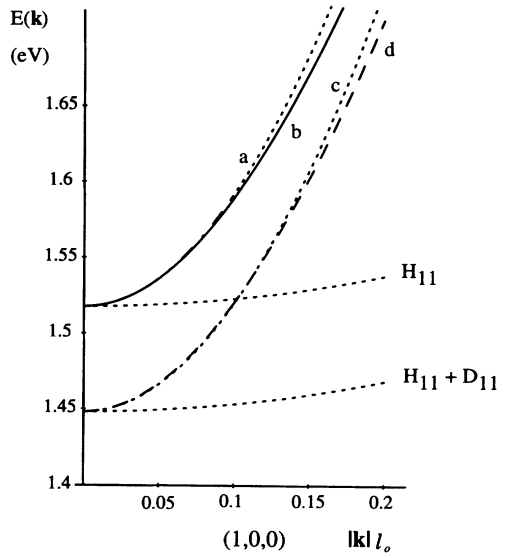

FIG. 2. The analytic conduction-band dispersion relations for GaAs (curves a and c) are compared with those calculated by numerically diagonalizing the eight-band model (curves b and d), for the unstrained (curves a and b) and biaxially strained (curves c and d) cases. The curves labeled H_{11} and $H_{11}+D_{11}$ show plots of the (1,1) matrix elements of H and $H+D$.

eight-band model for the case of zero and finite biaxial strain[22] are given by curves b and d, respectively. Curves a and c are plots of the analytic dispersion relations given in Eq. (4) for the case of zero strain and finite biaxial strain, respectively. The analytic expressions give a good representation of the dispersion for the conduction band. Note that the effective masses in curves a, b, c, and d are significantly smaller than the bare-electron mass. Mixing with the valence band is responsible for the reduced value of the conduction-band effective mass. The parameter values used for GaAs in the above plots are given in Table I.

IV. VALENCE BAND

The above renormalization procedure leads to a renormalized valence-band matrix $U_{\text{valence}}=U^{(0)}_{\text{valence}}+U^{(1)}_{\text{valence}}$, where the elements of $U^{(0)}_{\text{valence}}$ are independent of strain and the elements of $U^{(1)}_{\text{valence}}$ are linear in strain. Both matrices have the form

$$U_{\text{valence}}=-\begin{bmatrix} P-Q+b_1 & S^*+s^* & -R & t \\ S+s & P+Q+b_2 & 0 & -R \\ -R^* & 0 & P+Q+b_3 & -S^*-s_1^* \\ t^* & -R^* & -S-s_1 & P-Q+b_4 \end{bmatrix},$$

where the matrix elements s, s_1, t, b_1, b_2, b_3, and b_4 are linear in the parameter B (in the case of $U^{(0)}_{\text{valence}}$) and b' (in the case of $U^{(1)}_{\text{valence}}$). If inversion symmetry were present in the unstrained crystal, the band parameter B and deformation potential b' would both be identically zero.[9] The renormalized Hamiltonian matrix U_{valence} would then have O_h symmetry, appropriate for Ge or Si. In most instances the splitting due to inversion symmetry is believed to be small. For the case when $B=b'=0$, the renormalized valence-band matrix has the same symmetry as the Luttinger model and leads to doubly degenerate bands. For this case the renormalized valence-band matrix leads to dispersion relations that are given by

$$E_v=E_v^{(0)}+E_v^{(1)}\pm(E_k+E_{ks}+E_s)^{1/2}, \tag{9}$$

where

$$E_v^{(0)}=-\mathbf{k}^2\left[\frac{P_0^2}{3E_g}+\frac{\gamma_1}{2}\right]+(k_x^4+k_y^4+k_z^4)\left[\frac{\gamma_2^2}{\Delta}+\frac{P_0^2}{3E_g}\left[\frac{1}{2E_g}+\frac{A'}{E_g}+\frac{\gamma_1}{2E_g}+\frac{2\gamma_2}{\Delta}\right]\right]$$
$$+(k_x^2k_y^2+k_y^2k_z^2+k_x^2k_z^2)\left[\frac{3\gamma_3^2-\gamma_2^2}{\Delta}+\frac{P_0^2}{3E_g}\left[\frac{1}{E_g}+\frac{2A'}{E_g}+\frac{\gamma_1}{E_g}+\frac{6\gamma_3-2\gamma_2}{\Delta}\right]\right], \tag{10}$$

TABLE I. Eight-band model parameters used for plots of GaAs band structure.

Band Parameters						
γ_1^L	γ_2^L	γ_3^L	E_p (eV)	E_g (eV)	Δ (eV)	B
6.98[a]	2.25[a]	2.88[a]	22.7[b]	1.5177	0.341[c]	0[d]
Deformation-Potential Constants (eV)						
a'	b'	a	b	d		
−18.3[e]	0[d]	10[f]	−1.66[f]	−4.52[f]		
Strain (see Ref. 21)						
e_{xx}	e_{yy}	e_{zz}	e_{xy}	e_{xz}	e_{yz}	
3.5×10^{-3}	3.5×10^{-3}	-3.2×10^{-3}	0	0	0	

[a]M. S. Skolnick, A. K. Jain, R. A. Stradling, J. Leotin, J. C. Ousset, and S. Askenazy, J. Phys. C **9**, 2809 (1976).
[b]L. R. Ram-Mohan, K. H. Yoo, and R. L. Aggarwal, Phys. Rev. B **38**, 6151 (1988).
[c]*Semiconductors*, edited by O. Madelung, M. Schilz, and H. Weiss, Landolt-Börnstein, Numerical Data and Functional Relations in Science and Technology Vol. 17 (Springer-Verlag, New York, 1982).
[d]Doubly degenerate case chosen.
[e]A. Blacha, H. Presting, and M. Cardona, Phys. Status Solidi B **126**, 11 (1984).
[f]Fit to data of M. Chandrasekar and F. Pollak, Phys Rev. B **15**, 2127 (1977), assuming the value for $a'=-18.3$ eV, as given in footnote e.

$$E_v^{(1)}=-a(e_{xx}+e_{yy}+e_{zz})+(e_{xx}k_x^2+e_{yy}k_y^2+e_{zz}k_z^2)\left[\frac{P_0^2}{3E_g}\left[2+\frac{a'}{E_g}\right]-\frac{2b\gamma_2}{\Delta}\right]$$
$$+[(e_{yy}+e_{zz})k_x^2+(e_{xx}+e_{zz})k_y^2+(e_{xx}+e_{yy})k_z^2]\left[\frac{a'P_0^2}{3E_g^2}+\frac{b\gamma_2}{\Delta}\right]$$
$$+(e_{yz}k_yk_z+e_{xy}k_xk_y+e_{xz}k_xk_z)\left[\frac{4P_0^2}{3E_g}-\frac{2\sqrt{3}d\gamma_3}{\Delta}\right], \tag{11}$$

$$E_k=(k_x^2k_y^2+k_x^2k_z^2+k_y^2k_z^2)(\gamma_3-\gamma_2)\left[3(\gamma_3+\gamma_2)+\frac{2P_0^2}{E_g}\right]+(k_x^2+k_y^2+k_z^2)^2\left[\gamma_2^2+\frac{2\gamma_2P_0^2}{3E_g}+\frac{P_0^4}{9E_g^2}\right], \tag{12}$$

$$E_{ks}=\frac{b(3\gamma_2E_g+P_0^2)}{3E_g}[\mathbf{k}^2\mathrm{tr}(\overleftrightarrow{e})-3(k_x^2e_{xx}+k_y^2e_{yy}+k_z^2e_{zz})]$$
$$-2\sqrt{3}d\left[\gamma_3+\frac{P_0^2}{3E_g}\right](e_{xy}k_xk_y+e_{xz}k_xk_z+e_{yz}k_yk_z), \tag{13}$$

and

$$E_s=\frac{b^2}{2}[(e_{xx}-e_{yy})^2+(e_{xx}-e_{zz})^2+(e_{yy}-e_{zz})^2]$$
$$+d^2(e_{xy}^2+e_{xz}^2+e_{yz}^2). \tag{14}$$

In Eq. (9), the term E_k depends only on wave vectors and E_s depends only on strain. The cross terms are contained in E_{ks} and we have dropped terms in E_{ks} higher than first order in strain and second order in wave vector. In the absence of strain the plus (minus) sign corresponds to the heavy (light) hole.

In the limit of large valence-to-conduction-band gap, $E_g\rightarrow\infty$, and large spin-orbit band gap $\Delta\rightarrow\infty$, Eq. (9) reproduces the results of Pikus and Bir,[1] who used a Luttinger model which does not include mixing with the conduction and spin-orbit bands (see Appendix B). Their expression does not contain the quartic wave vector and band warping terms contained in Eq. (10). The Pikus-Bir (PB) result contains only the coupling to hydrostatic deformations, corresponding to the first term in Eq. (11). When band mixing is included, the Pikus-Bir band constants A_{PB}, B_{PB}, and C_{PB} are renormalized by terms proportional to P_0, $1/E_g$, and $1/\Delta$, that result from band mixing. Note, however, that the deformation-potential constants a, b, and d are not renormalized when band mixing is included.

Figure 3 shows the strained and unstrained hole bands as calculated by numerically diagonalizing the eight-band model. The characteristic effect of light mass along the (1,0,0) direction and heavy mass along the (0,0,1) direction can be seen in the strained (dashed) curves. Figure 4 shows a comparison of the analytic results (dashed curves), given by Eq. (9), with those obtained by numerical diagonalization of the eight-band model (solid curves), for the case of zero strain, along the (1,0,0) and (1,1,1) **k**-space directions. The analytic results give a good approximation along the (1,0,0) direction for both the light and heavy hole but the approximation is not as good along the (1,1,1) direction for heavy hole. Figure 5 shows a comparison of the analytic and numerical results for the biaxially strained case, along (1,0,0) and (0,0,1) **k**-space directions. Finally, Fig. 6 shows the same comparison along the (1,1,1) direction.

V. SPIN-ORBIT BAND

Using the above renormalization procedure, we calculate the second-renormalized matrix for the spin-orbit split-off band, $U_{\mathrm{s.o.}}=U_{\mathrm{s.o.}}^{(0)}+U_{\mathrm{s.o.}}^{(1)}$, where the elements of $U_{\mathrm{s.o.}}^{(0)}$ are correct to quadratic order in wave-vector components and elements of $U_{\mathrm{s.o.}}^{(1)}$ are correct to linear terms in strain and quadratic terms in wave vector. This leads to dispersion relations given by

$$E_{\mathrm{s.o.}}=(E_{\mathrm{s.o.}}^{(0)}+E_{\mathrm{s.o.}}^{(1)})(1\pm\delta\varepsilon_{\mathrm{s.o.}}), \tag{15}$$

where

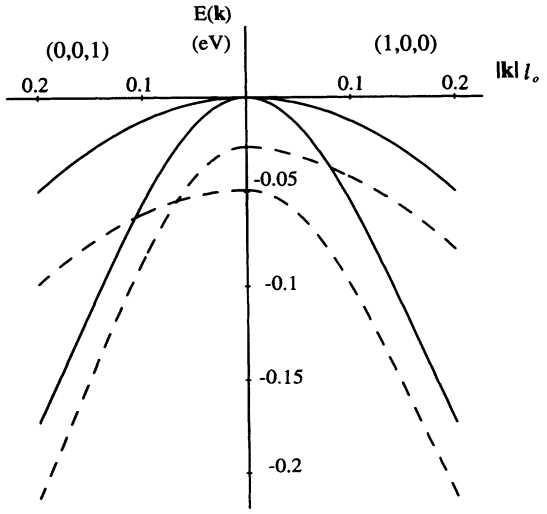

FIG. 3. The valence band of GaAs, as calculated by diagonalizing the eight-band model, is shown for the case of zero strain (solid curves) and biaxial strain (dashed curves) along the (1,0,0) and (0,0,1) **k**-space directions.

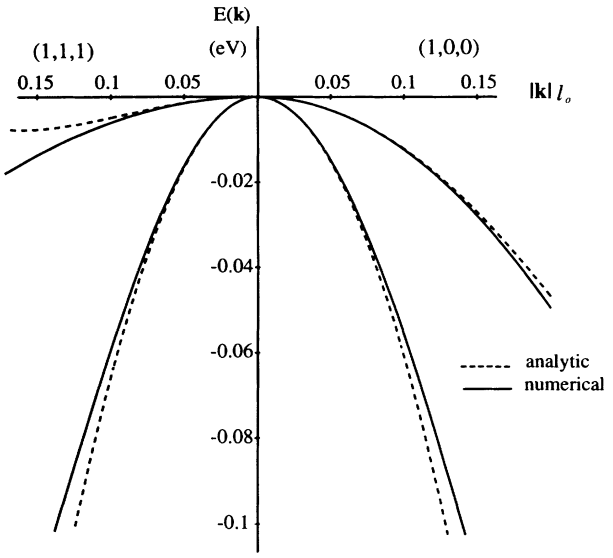

FIG. 4. The analytic dispersion relations (dotted curves) for the valence band of unstrained GaAs are compared with those calculated from the eight-band model by numerical diagonalization (solid curves).

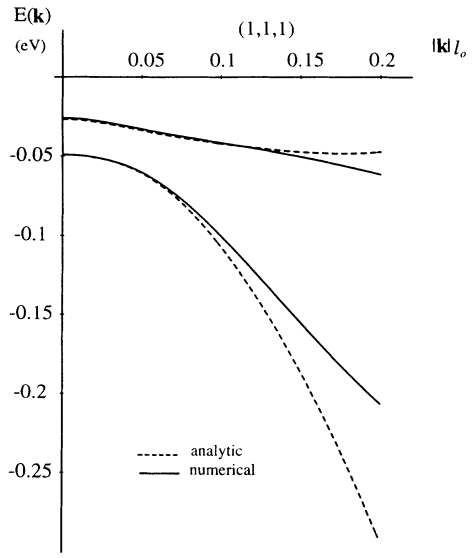

FIG. 6. The analytic dispersion relations for the valence band of biaxially strained GaAs (dotted curves) are compared with those calculated from the eight-band model by numerical diagonalization (solid curves) along the (1,1,1) **k**-space direction.

$$E_{\text{s.o.}}^{(0)} = -\Delta - \left[\frac{\gamma_1}{2} + \frac{P_0^2}{3(E_g+\Delta)}\right]\mathbf{k}^2 , \tag{16}$$

$$E_{\text{s.o.}}^{(1)} = -\left[a + \left[\frac{2b\gamma_2}{\Delta} - \frac{a'P_0^2}{3(E_g+\Delta)^2}\right]\mathbf{k}^2\right]\text{tr}(\overleftrightarrow{e}) + \left[\frac{6b\gamma_2}{\Delta} + \frac{2P_0^2}{3(E_g+\Delta)}\right](e_{xx}k_x^2 + e_{yy}k_y^2 + e_{zz}k_z^2)$$
$$+ (e_{xy}k_xk_y + e_{yz}k_yk_z + e_{xz}k_xk_z)\left[\frac{4\sqrt{3}d\gamma_3}{\Delta} + \frac{4P_0^2 - 2Bb'}{3(E_g+\Delta)}\right] , \tag{17}$$

$$\delta\varepsilon_{\text{s.o.}}^{(1)} = \frac{2}{3}\left|\frac{b'P_0}{E_g+\Delta}\right|[(e_{xy}^2+e_{xz}^2)k_x^2 + (e_{xy}^2+e_{yz}^2)k_y^2 + (e_{xz}^2+e_{yz}^2)k_z^2 - 2e_{xz}e_{yz}k_xk_y - 2e_{xy}e_{yz}k_xk_z - 2e_{xy}e_{xz}k_yk_z]^{1/2} . \tag{18}$$

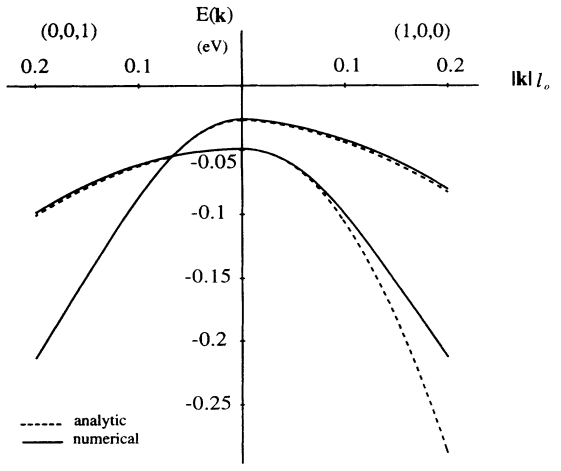

FIG. 5. The analytic dispersions (dotted curves) for the valence band of biaxially strained GaAs are compared with those calculated from the eight-band model by numerical diagonalization (solid curves).

In the absence of strain, the mass of the spin-orbit band is isotropic. When strain is present (e.g., biaxial strain), an asymmetry in the masses is introduced as a result of the strain, coming from $E_{\text{s.o.}}^{(1)}$. Figure 7 shows the comparison of the dispersion relations given by the analytic expression in Eq. (15) and that observed by numerical diagonalization of the eight-band model, for the biaxially strained and unstrained cases.

VI. CONCLUSION

An eight-band model of energy bands in the vicinity of $\mathbf{k}=\mathbf{0}$ is believed to give accurate dispersion relations in the presence of small (but arbitrary) strain. Due to the size of the 8×8 matrix $U=H+D$, in general these relations must be calculated numerically. We have obtained analytic approximations to the dispersion relations of the eight-band model by performing a second Löwdin renormalization on the matrix U, to obtain "second-renormalized matrices" of smaller dimensions, 2×2,

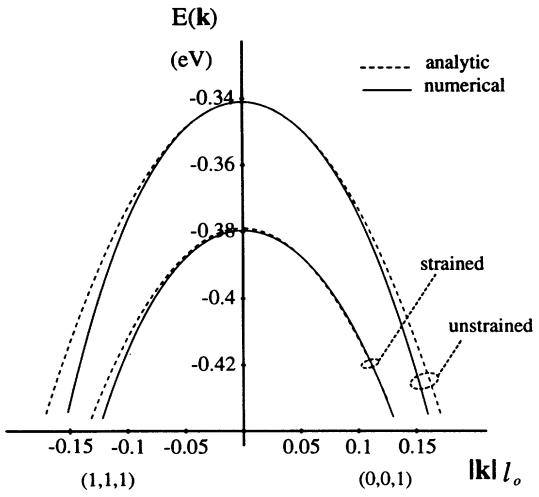

FIG. 7. The analytic spin-orbit split-off band dispersions for GaAs (dotted curves) are compared with those calculated by numerically diagonalizing the eight-band model for the unstrained and biaxially strained cases.

4×4, and 2×2, for the conduction, light- and heavy-hole, and spin-orbit bands, respectively. The reduced dimensionality of these matrices allows us to obtain analytic dispersion relations for the conduction, light- and heavy-hole, and spin-orbit bands, in the presence of a small but arbitrary strain. Our primary results are given by Eqs. (4)–(18). Comparison of the analytic dispersions to those obtained by numerically diagonalizing the eight-band model shows that the analytic dispersions give a reasonable approximation near $\mathbf{k}=\mathbf{0}$.

Our results are appropriate for the zinc-blende group of semiconductors which have a direct energy gap at $\mathbf{k}=\mathbf{0}$ for which the small point group of $\mathbf{k}$ at $\mathbf{k}=0$ is T_d (which lacks inversion symmetry). Our results in Eq. (9)–(18) for the light- and heavy-hole and spin-orbit bands apply equally well to the case of Si and Ge which have O_h symmetry (and have inversion symmetry), if we take $B=b'=0$ and $P_0=0$. In the eight-band model we simply neglect the conduction-band block. This leads to a six-band model without a conduction band.

The renormalization scheme we have used is quite general and consequently can be applied to other many-band $\mathbf{k}\cdot\mathbf{p}$ models to derive analytic dispersion relations.

ACKNOWLEDGMENT

I thank John D. Bruno for many helpful discussions.

APPENDIX A: THE MATRICES H AND D

The matrix H is given by

$$H=\begin{array}{c|cccccc}
 & \Gamma_{-1/2}^{6} & \Gamma_{1/2}^{6} & U_{-3/2}^{\Gamma_8} & \Gamma_{-1/2}^{8} & \Gamma_{1/2}^{8} & \Gamma_{3/2}^{8} & \Gamma_{-1/2}^{7} & \Gamma_{1/2}^{7} \\
\hline
\Gamma_{-1/2}^{6} & A & 0 & T^*+V^* & 0 & -\sqrt{3}(T-V) & \sqrt{2}(W-U) & W-U & \sqrt{2}(T^*+V^*) \\
\Gamma_{1/2}^{6} & 0 & A & \sqrt{2}(W-U) & -\sqrt{3}(T^*+V^*) & 0 & T-V & -\sqrt{2}(T-V) & W^*+U \\
U_{-3/2}^{\Gamma_8} & T+V & \sqrt{2}(W^*-U) & -P+Q & -S^* & R & 0 & (\tfrac{3}{2})^{1/2}S & -\sqrt{2}Q \\
\Gamma_{-1/2}^{8} & 0 & -\sqrt{3}(T+V) & -S & -P-Q & 0 & R & -\sqrt{2}R & \frac{1}{\sqrt{2}}S \\
\Gamma_{1/2}^{8} & -\sqrt{3}(T^*-V^*) & 0 & R^* & 0 & -P-Q & S^* & \frac{1}{\sqrt{2}}S^* & \sqrt{2}R^* \\
\Gamma_{3/2}^{8} & \sqrt{2}(W^*-U) & T^*-V^* & 0 & R^* & S & -P+Q & \sqrt{2}Q & (\tfrac{3}{2})^{1/2}S^* \\
\Gamma_{-1/2}^{7} & W^*-U & -\sqrt{2}(T^*-V^*) & (\tfrac{3}{2})^{1/2}S^* & -\sqrt{2}R^* & \frac{1}{\sqrt{2}}S & \sqrt{2}Q & Z & 0 \\
\Gamma_{1/2}^{7} & \sqrt{2}(T+V) & W+U & -\sqrt{2}Q & \frac{1}{\sqrt{2}}S^* & \sqrt{2}R & (\tfrac{3}{2})^{1/2}S & 0 & Z
\end{array}, \tag{A1}$$

where

$$A=E_c+\left[A'+\frac{\hbar^2}{2m_0}\right](k_x^2+k_y^2+k_z^2)\ ,$$

$$P=-E_v+\tfrac{1}{2}\gamma_1\frac{\hbar^2}{m_0}(k_x^2+k_y^2+k_z^2)\ ,$$

$$U=\frac{1}{\sqrt{3}}P_0k_z\ ,\quad Q=\tfrac{1}{2}\gamma_2\frac{\hbar^2}{m_0}(k_x^2+k_y^2-2k_z^2)\ ,$$

$$V=\frac{1}{\sqrt{6}}P_0(k_z-ik_y)\ ,$$

$$R=-\frac{\sqrt{3}}{2}\frac{\hbar^2}{m_0}[\gamma_2(k_x^2-k_y^2)-2i\gamma_3k_xk_y]\ , \tag{A2}$$

$$W=i\frac{1}{\sqrt{3}}Bk_xk_y+,\quad S=\sqrt{3}\gamma_3\frac{\hbar^2}{m_0}k_z(k_x-ik_y)\ ,$$

$$T=\frac{1}{\sqrt{6}}Bk_z(k_x+ik_y)\ ,$$

$$Z=E_v-\Delta-\tfrac{1}{2}\gamma_1\frac{\hbar^2}{m_0}(k_x^2+k_y^2+k_z^2)\ .$$

The constants γ_1, γ_2, and γ_3 are the modified Luttinger parameters, and are the related to the parameters used by Luttinger,[15] γ_1^L, γ_2^L, and γ_3^L, by

$$\gamma_1=\gamma_1^L-\frac{E_P}{3E_g+\Delta}\ ,$$

$$\gamma_2=\gamma_2^L-\frac{1}{2}\frac{E_P}{3E_g+\Delta}\ , \tag{A3}$$

$$\gamma_3=\gamma_3^L-\frac{1}{2}\frac{E_P}{3E_g+\Delta}\ ,$$

where the conduction- to valence-band gap

$$E_g=E_c-E_v \tag{A4}$$

and the conduction-valence mixing parameter E_P is related to the valence-band–conduction-band momentum matrix element P_0 by

$$E_P=\frac{2m_0}{\hbar^2}P_0^2\ . \tag{A5}$$

In Eq. (16), the constant A' results from the interaction of the Γ_6 conduction band with class-B states (outside the eight-dimensional manifold of class-A states). The matrix H does not include the linear-$\mathbf{k}$ terms which have been shown to be negligible for most purposes.[11,12]

The matrix D is given by

$$D=\begin{array}{c|cccccccc}
 & \Gamma_6 & \Gamma_6 & \Gamma_8 & \Gamma_8 & \Gamma_8 & \Gamma_8 & \Gamma_7 & \Gamma_7 \\
 & u_{-1/2} & u_{1/2} & u_{-3/2} & u_{-1/2} & u_{1/2} & u_{3/2} & u_{-1/2} & u_{1/2} \\
\hline
\Gamma_6\ u_{-1/2} & a'e & 0 & t^*-v^* & 0 & -\sqrt{3}(t+v) & \sqrt{2}(w+u) & w+u & \sqrt{2}(t^*-v^*) \\
\Gamma_6\ u_{1/2} & 0 & a'e & \sqrt{2}(w+u) & -\sqrt{3}(t^*-v^*) & 0 & t+v & -\sqrt{2}(t+v) & w^*-u \\
\Gamma_8\ u_{-3/2} & t-v & \sqrt{2}(w^*+u) & -p+q & -s^* & r & 0 & (\tfrac{3}{2})^{1/2}s & -\sqrt{2}q \\
\Gamma_8\ u_{-1/2} & 0 & -\sqrt{3}(t-v) & -s & -p-q & 0 & r & -\sqrt{2}r & \frac{1}{\sqrt{2}}s \\
\Gamma_8\ u_{1/2} & -\sqrt{3}(t^*+v^*) & 0 & r^* & 0 & -p-q & s^* & \frac{1}{\sqrt{2}}s^* & \sqrt{2}r^* \\
\Gamma_8\ u_{3/2} & \sqrt{2}(w^*+u) & t^*+v^* & 0 & r^* & s & -p+q & \sqrt{2}q & (\tfrac{3}{2})^{1/2}s^* \\
\Gamma_7\ u_{-1/2} & w^*+u & -\sqrt{2}(t^*+v^*) & (\tfrac{3}{2})^{1/2}s^* & -\sqrt{2}r^* & \frac{1}{\sqrt{2}}s & \sqrt{2}q & -ae & 0 \\
\Gamma_7\ u_{1/2} & \sqrt{2}(t-v) & w-u & -\sqrt{2}q & \frac{1}{\sqrt{2}}s^* & \sqrt{2}r & (\tfrac{3}{2})^{1/2}s & 0 & -ae
\end{array}\ , \tag{A6}$$

where

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

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

$$u=\frac{1}{\sqrt{3}}P_0\sum_j e_{zj}k_j\ ,\quad r=\frac{\sqrt{3}}{2}b(e_{xx}-e_{yy})-ide_{xy}\ , \tag{A7}$$

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

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

The Pikus and Bir[1] deformation-potential constants a, b, and d describe the coupling of the valence band to strain while the constants a' and b' describe the coupling of the conduction band to strain.[9]

APPENDIX B: COMPARISON WITH PIKUS AND BIR

Pikus and Bir have derived dispersion relations for the valence band appropriate for O_h group symmetry (the case of Si and Ge).[1] They used a Luttinger model with strain interactions, and assumed that the spin-orbit splitting Δ and the conduction-band–valence-band gap E_g were arbitrarily large, so that there is no mixing of the valence bands with the conduction or spin-orbit bands. They found that the two doubly degenerate bands can be given as (with energy taken to be negative)

$$E_{1,2}=-A_{\rm PB}\mathbf{k}^2-a\ \mathrm{tr}(\overleftrightarrow{e})\pm(\varepsilon_k+\varepsilon_{ks}+\varepsilon_s)^{1/2}\ , \tag{B1}$$

where

$$\varepsilon_k=B_{\rm PB}^2(k_x^2+k_y^2+k_z^2)^2+C_{\rm PB}^2(k_x^2k_y^2+k_x^2k_z^2+k_y^2k_z^2)\ , \tag{B2}$$

$$\varepsilon_s=\frac{b^2}{2}[(e_{xx}-e_{yy})^2+(e_{xx}-e_{zz})^2+(e_{yy}-e_{zz})^2]+d^2(e_{xy}^2+e_{xz}^2+e_{yz}^2)\ , \tag{B3}$$

$$\varepsilon_{ks}=bB_{\rm PB}[3(k_x^2e_{xx}+k_y^2e_{yy}+k_z^2e_{zz})-\mathbf{k}^2\mathrm{tr}(\overleftrightarrow{e})]+2dD_{\rm PB}(e_{xy}k_xk_y+e_{yz}k_yk_z+e_{xz}k_xk_z)\ , \tag{B4}$$

and

$$A_{\rm PB}=-\left[\frac{L+2M}{3}+\frac{\hbar^2}{2m_0}\right]=\frac{\hbar^2}{2m_0}\gamma_1^L\ , \tag{B5}$$

$$B_{\rm PB}=\frac{L-M}{3}=-\frac{\hbar^2}{m_0}\gamma_2^L\ , \tag{B6}$$

$$D_{\rm PB}=\frac{N}{\sqrt{3}}=-\sqrt{3}\frac{\hbar^2}{m_0}\gamma_3^L\ , \tag{B7}$$

$$C_{\rm PB}^2=D_{\rm PB}^2-3B_{\rm PB}^2=3\left[\frac{\hbar^2}{m_0}\right]^2[(\gamma_3^L)^2-(\gamma_2^L)^2]\ . \tag{B8}$$

The parameters γ_1^L, γ_2^L, and γ_3^L are the Luttinger parameters and $A_{\rm PB}$, $B_{\rm PB}$, $D_{\rm PB}$, and $C_{\rm PB}$ are the Pikus-Bir band parameters.[1]

[1] G. E. Pikus and G. L. Bir, Fiz. Tverd. Tela (Leningrad) **1**, 1642 (1960) [Sov. Phys. Solid State **1**, 1502 (1960)].

[2] See also G. L. Bir and G. E. Pikus, *Symmetry and Strain-Induced Effects in Semiconductors* (Wiley, New York, 1974).

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[14] We use the notation in G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, *Properties of the Thirty-Two Point Groups* (MIT Press, Cambridge, 1963).

[15] J. M. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1955); J. M. Luttinger, *ibid.* **102**, 1030 (1956).

[16] The original strain-independent eight-band model H is correct only to terms $O(k_i^2)$. However, fourth-order terms that couple the conduction-band states via intermediate valence-band states are zero, since $\langle v_i|\mathbf{k}\cdot\mathbf{p}|v_j\rangle=0$, where v_i are the class-A valence-band states at $\mathbf{k}=0$ in the original eight-band model. There are nonzero fourth-order terms which couple the conduction-band states via class-B states (in the original eight-band model), but these are small because of the large energy denominators between the conduction-band states at $\mathbf{k}=\mathbf{0}$ and the class-B states.

[17] The original strain-independent eight-band model H neglects the small linear-$\mathbf{k}$ terms which may be important in the immediate vicinity of the zone center (see Ref. 11). The condition on the perturbation expansion then means that we must restrict our attention to wave vectors slightly away from $\mathbf{k}=\mathbf{0}$.

[18] S. Wolfman, *Mathematica a System for Doing Mathematics by Computer* (Addison-Wesley, New York, 1991).

[19] We represent strain by the strain tensor, $e_{ij}=\frac{1}{2}(\partial v_i/\partial x_j+\partial v_j/\partial x_i)$, where $v_i=x_i'-x_i=e_{ij}x_j$ are the displacement field components.

[20] Throughout this work, except Appendix B, we use units such that $\hbar=m_0=1$, where m_0 is the bare electron mass. To restore these constants, make the following replacements: $k_i\rightarrow(\hbar/\sqrt{m_0})k_i$, $P_0\rightarrow(\sqrt{m_0}/\hbar)P_0$, $B\rightarrow(m_0/\hbar^2)B$, and $A'\rightarrow(m_0/\hbar^2)A'$.

[21] D. L. Smith and C. Mailhiot, Rev. Mod. Phys. **62**, 173 (1990).

[22] The strain chosen in the illustrations is roughly that which a thin layer of GaAs would experience when grown epitaxially between bulk layers of $Ga_xIn_{1-x}P$ for $x\approx0.5$.