Analytical approach to the inversion-asymmetry splitting of the valence band in zinc-blende-type semiconductors

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We have extended the model that we developed earlier for the analytical extraction of the eigenvalues of the $\mathbf{k}\cdot\mathbf{p}$ matrix [Phys. Rev. B **42**, 7513 (1990)] to account for large matrices. We then applied this to the 8×8 matrix of the zinc-blende-type semiconductors. We manage to extract analytical expansion for the energies of the valence bands as well as the conduction band as a function of the wave vector $\mathbf{k}$ in a general direction up to third order. Simple expressions for the first-, second-, and third-order terms were obtained in terms of k_x, k_y, and k_z together with the band parameters.

I. INTRODUCTION

There is a growing interest in the energy wave-vector expansion of the band structure of semiconductors close to the band edge.[1–8] In spite of the fact that the contribution of the asymmetry splitting terms in this expansion is very small, they are responsible for so many interesting experimental phenomena. Second-harmonic generation, optical rectification, spin-relaxation time which can be measured by means of the Hanle effect,[9–11] and other forms of polarized luminescence[12,13] are among these phenomena. The cubic term in this expansion also affects the strength of the electric-field-induced spin resonance and, based on this fact, this term has been determined in InSb.[14,15] The spin splitting of the bands of GaAs along $\langle 110\rangle$ has also been observed in the spin-polarized photoemission experiments of Riechert *et al.*[16] Moreover, splittings linear in the wave vector $\mathbf{k}$ are often induced by application of uniaxial stress.[17] Such splitting can also be observed by means of the Hanle effect.[11] An explicit form of the k^3 term of the conduction band has been calculated by Braun and Rossler[3] and by Christensen and Cardona.[1] This term was also calculated at the $\langle 110\rangle$ $\mathbf{k}$ direction in the comprehensive work presented by Cardona, Christensen, and Fasol.[4] However, no attempt has been made to calculate these terms for the valence band in the general direction of the wave vector $\mathbf{k}$.

In a recent paper,[18] we have introduced an analytical technique for extracting the energy wave-vector expansion from the $\mathbf{k}\cdot\mathbf{p}$ (Ref. 19) matrix. It was then successfully applied to get all the roots of the 7×7 matrix representing the band structure of Ge (Ref. 20) at $\mathbf{k}$ in the z direction. In order to apply this technique, an explicit form of the secular equation of the matrix is needed. However, this secular equation is not always easy to obtain in an explicit form. For instance, in the case of the four-band model for zinc-blende-type semiconductors the secular equation of the resulting 8×8 $\mathbf{k}\cdot\mathbf{p}$ matrix, taking the vector $\mathbf{k}$ in a general direction, contains around forty-thousand terms (8!) which are almost impossible to express in an explict form.

The aim of this work is to extend the model to be applied on large matrices without the need for the full explicit form of the secular equation. In this case, we can extract only the terms which are needed for certain calculations directly from the matrix itself. We will then obtain the energy wave-vector expansion for all the bands up to third order. In our derivation we will adopt the four-band model given by Trebin, Rossler, and Ranvaud.[21] The 8×8 $\mathbf{k}\cdot\mathbf{p}$ matrix represents the lowest twofold degenerate conduction band Γ_6, the uppermost fourfold degenerate valence band Γ_8^v, and the twofold degenerate split-off band Γ_7^v. In the case of the Γ_6 conduction band the perturbation method can be used to get its energy wave-vector expansion, since the secular equation will end up to be that of a 2×2 matrix which can easily be solved.[3] However, for the case of the Γ_8^v valence band the perturbation theory will lead to a 4×4 matrix for which the secular equation cannot be solved analytically. Only our technique in this case is capable of producing this expansion up to the desired order.

Our work is organized as follows. The model with the extension that accounts for the large matrices is presented in Sec. II. The application is given in Sec. III and a discussion of the results is given in Sec. IV. Section V is the conclusion.

II. THE MODEL

According to Ref. 18 the z surface root (the root that goes to zero with vanishing z) of the polynomial equation

$$\sum_{n=0}^{k} P_n(z)X^n=0 \tag{1}$$

can be given by

$$X=\sum_{n=1}^{\infty} a_n z^n\ , \tag{2}$$

where the coefficients a_n can be obtained from the set of equations

$$P_0^{[m]}+\sum_{s=1}^{m}\sum_{n=1}^{\min(s,k)} P_n^{[m-s]}F_n^s\{a_i\}=0 \tag{3}$$

with

$$P_n^{[m]}=\frac{1}{m!}\left[\frac{d^m P_n(z)}{dz^m}\right]_{z=0}\ , \tag{4}$$

and $F_n^s\{a_i\}$ is a function of the set $\{a_i\}$ defined as the sum of all the possible permutations of the product of n members of the set $\{a_i\}$ such that the sum of their subscript is equal to s. The first few equations of the set (3) are shown in Ref. 18. These equations can be solved one by one to get a_i up to the desired order. From these equations we can see that we only need the values of $P_n^{[m]}$ from the secular equation in order to get a_i up to the desired order. In the following we will see how these values can be obtained directly from the matrix itself.

It is well known that the secular equation of the matrix $[c_{ij}(x)]$ can be expressed by Eq. (1) with $P_n(z)$ having the form

$$P_n(z)=(-1)^{k-n}S_{k-n}(z) , \tag{5}$$

where

$$S_0(z)=1 , \quad S_1(z)=\mathrm{tr}[c_{ij}(z)] , \quad S_k(z)=\det[c_{ij}(z)] , \tag{6}$$

and $S_m(z)$ $(m=2,3,\ldots,k-1)$ is the sum of all the m-square principal minors of $[c_{ij}(z)]$. Now we have

$$P_n^{[m]}=(-1)^{k-n}S_{k-n}^{[m]} , \tag{7}$$

where

$$S_l^{[m]}=\frac{1}{m!}\left[\frac{d^m S_l(z)}{dz^m}\right]_{z=0} . \tag{8}$$

III. APPLICATION OF THE MODEL

To apply the model to the 8×8 matrix given by Table IV of Ref. 21 we will take $z=k$ and assume that at $k=0$ the Γ_6 conduction band is situated at the energy value A_1, the Γ_8^v valence band at A_2 (separated from A_1 by the band gap E_0), and the Γ_7^v split-off valence band at A_3 (separated from A_2 by the spin-orbit splitting Δ). The origin of the energy scale will be taken arbitrarily according to the band we want to obtain. In the following the band parameters P, B, C, and A' are defined in Ref. 21. The parameters γ_1, γ_2, and γ_3 are related to the Luttinger parameters γ_{1L}, γ_{2L}, and γ_{3L} by the following relations:

$$\gamma_{1L}=\gamma_1+\frac{P^2}{3E_0} , \quad \gamma_{2L}=\gamma_2+\frac{P^2}{6E_0} , \quad \gamma_{3L}=\gamma_3+\frac{P^2}{6E_0} .$$

A. Energies of the Γ_8^v valence band

Now, to get the energies of the Γ_8^v valence band we will choose the following:

$$A_1=E_0 , \quad A_2=0 , \quad A_3=-\Delta . \tag{9}$$

In this case, we have

$$P_1(0)=0 , \quad P_2(0)=0 , \quad P_3(0)=0 , \quad P_0^{[2]}=0 , \quad P_1^{[2]}=0 . \tag{10}$$

Hence, the first nontrivial equation of the set (3) is

$$P_0^{[4]}+P_2^{[2]}a_1^2+P_4(0)=0 . \tag{11}$$

Now, using Eq. (7) we get

$$P_4(0)=A_1^2A_3^2 , \quad P_2^{[2]}=-2C^2A_1^2A_3^2 , \quad P_0^{[4]}=C^4(1-3S)A_1^2 , \tag{12}$$

where

$$S=(k_y^2k_z^2+k_z^2k_x^2+k_x^2k_y^2)/k^4 . \tag{13}$$

Substituting in Eq. (11) we get

$$a_1^4-2C^2a_1^2+C^4(1-3S)=0 ,$$

which gives for a_1

$$a_1=\pm C(1\pm\sqrt{3S}\,)^{(1/2)} . \tag{14}$$

This form is identical with that obtained by Dresselhaus.[22] Now, to simplify the derivation of the higher-order terms, we will set $C=0$. Hence, the next nontrivial equation will be

$$P_0^{[8]}+P_1^{[6]}a_2+P_2^{[4]}a_2^2+P_3^{[2]}a_2^3+P_4(0)a_2^4=0 , \tag{15}$$

where

$$P_3^{[2]}=2A_1^2A_3^2s_1 , \quad P_2^{[4]}=A_1^2A_3^2(2s_0+s_1^2) , \quad P_1^{[6]}=2A_1^2A_3^2s_0s_1 , \quad P_0^{[8]}=A_1^2A_3^2s_0 \tag{16}$$

with

$$s_0=\gamma_1^2-s^2+2\gamma_0(2\gamma_1-t) , \quad s_1=2(\gamma_1+2\gamma_0) , \quad \gamma_0=\frac{p^2}{6A_1^2} , \quad s^2=4[\gamma_2^2+3(\gamma_3^2-\gamma_2^2)S] , \quad t=4[\gamma_2+3(\gamma_3-\gamma_2)S] . \tag{17}$$

By using Eqs. (16) and (17) we see that Eq. (15) can be factorized to become

$$(a_2^2+s_1a_2+s_0)^2=0 . \tag{18}$$

This yields for a_2

$$a_2=-(\gamma_1+2\gamma_0)\pm(\gamma_0^2+s^2+\gamma_0t)^{1/2} \tag{19}$$

using the notation

$$s_L^2=4[\gamma_{2L}^2+3(\gamma_{3L}^2-\gamma_{2L}^2)S] . \tag{20}$$

Equation (19) can be reduced to

$$a_2=-\gamma_{1L}\pm s_L \tag{21}$$

with a positive singe for the heavy-hole and a negative singe for the light-hole valence bands. Equation (21) gives for a_2 an identical expression with the well-known Luttinger[23] one.

The equation from the set (3) which gives the expression for a_3 is

$$P_0^{[10]}+P_1^{[8]}a_2+P_2^{[6]}a_2^2+P_3^{[4]}a_2^3+P_2^{[4]}a_3^2+P_4^{[2]}a_2^4+3P_3^{[2]}a_2a_3^2+P_5(0)a_2^5+6P_4(0)a_2^2a_3^2=0 \tag{22}$$

which yields

$$a_3=\pm\frac{2PB(S-9T)^{1/2}}{3E_0s_L}\left\{\gamma_{2L}(2\gamma_{2L}\mp s_L)+6(\gamma_{3L}-\gamma_{2L})\left[\gamma_{2L}S+(2\gamma_{3L}\mp s_L)\frac{(S^2-3T)}{(S-9T)}\right]\right\}^{1/2}, \tag{23}$$

where

$$T=(k_x^2k_y^2k_z^2)/k^6 . \tag{24}$$

B. The energy of the Γ_7^v split-off valence band

To get the energy of the Γ_7^v split-off valence band we will choose

$$A_1=E_0+\Delta , \quad A_2=\Delta , \quad A_3=0 \tag{25}$$

which by using Eq. (7) gives

$$P_1(0)=0 , \quad P_0^{[2]}=0 . \tag{26}$$

The first nontrivial equation will then be

$$P_0^{[2]}+P_1(0)a_2+P_2(0)a_1^2=0 \tag{27}$$

with

$$P_2(0)=A_1^2A_2^2 . \tag{28}$$

Equation (27) gives

$$a_1=0 . \tag{29}$$

Setting $a_1=0$ (we will also set $C=0$), the next equation will be

$$P_0^{[4]}+P_1^{[2]}a_2+P_2(0)a_2^2=0 , \tag{30}$$

where

$$P_1^{[2]}=2A_1^2A_2^2\left[\gamma_1+\frac{P^2}{3A_1}\right], \tag{31}$$

$$P_0^{[4]}=A_1^2A_2^2\left[\gamma_1+\frac{p^2}{3A_1}\right]^2 . \tag{32}$$

Using Eqs. (28), (31), (32), and (25), Eq. (30) will yield for a_2 the expression

$$a_2=-\left[\gamma_1+\frac{P^2}{3(E_0+\Delta)}\right] . \tag{33}$$

This is identical with the well-known form of a_2 for the Γ_7^v split-off valence band.

The equation for a_3 is

$$P_0^{[6]}+P_1^{[4]}a_2+P_2^{[2]}a_2^2+P_2(0)a_3^2=0 \tag{34}$$

which yields

$$a_3=\pm\tfrac{2}{3}\frac{PB}{(E_0+\Delta)}(S-9T)^{1/2} . \tag{35}$$

C. The energy of the Γ_6 conduction band

The case of the Γ_6 conduction band has been studied previously[3] but will be considered here for completeness. In this case, we will set

$$A_1=0 , \quad A_2=-E_0 , \quad A_3=-(E_0+\Delta) . \tag{36}$$

All the arguments we have for the Γ_7^v split-off valence band are applicable to the case of the Γ_6 conduction band. Hence, Eqs. (28), (31), and (32) will be replaced by

$$P_2(0)=A_3^2A_2^4 , \tag{37}$$

$$P_1^{[2]}=-2A_3^2A_2^4\left\{\frac{\hbar^2}{2m}+A'-\frac{P^2}{3}\left[\frac{2}{A_2}+\frac{1}{A_3}\right]\right\}, \tag{38}$$

$$P_0^{[4]}=A_3^2A_2^4\left\{\frac{\hbar^2}{2m}+A'-\frac{P^2}{3}\left[\frac{2}{A_2}+\frac{1}{A_3}\right]\right\}^2 . \tag{39}$$

Now using Eqs. (37)–(39) we get from Eqs. (27), (30), (34), and (36) for the Γ_6 conduction band

$$a_1=0 , \tag{40}$$

$$a_2=\frac{\hbar^2}{2m}+A'+\frac{P^2}{3}\left[\frac{2}{E_0}+\frac{1}{E_0+\Delta}\right], \tag{41}$$

$$a_3=\pm\tfrac{2}{3}PB\left[\frac{1}{E_0}-\frac{1}{E_0+\Delta}\right](S-9T)^{1/2} . \tag{42}$$

IV. DISCUSSION OF THE RESULTS

As we saw, the extended model has been successful in leading to the derivation of the energy wave-vector expansion for the case of the four-band model represented by the 8×8 $\mathbf{k}\cdot\mathbf{p}$ matrix. It gives for the Γ_8^v valence band linear and quadratic terms which are identical with the published ones. For third-order terms the only attempt to calculate these terms was made by Cardona, Christensen, and Fasol[4] by applying third-order perturbation theory on the 14×14 $\mathbf{k}\cdot\mathbf{p}$ matrix and taking the wave vector $\mathbf{k}$ in the $\langle 110\rangle$ direction. Their result agrees with that of Eq. (23) up to first order in $(\gamma_3-\gamma_2)$. However, our result (limited to the four-band model) is more accurate since the extraction of these third-order terms from the matrix is complete with no perturbative approximations. For the case of the Γ_7^v valence band the first- and second-order terms agree with the well-known published data. The third-order term was also calculated by Cardo-

na, Christensen, and Fasol[4] in the $\langle 110 \rangle$ **k** direction. Limited to the four-band model, their result is in agreement with ours.

The conduction band has been extensively studied by perturbation theory.[1–4] Our result agrees completely with the published data for all the calculated terms. For example, Braun and Rossler[3] obtained for the third-order term,

$$a_3 = \pm \frac{2PP'Q}{3} \left\{ \frac{\Delta}{E_0(E_0+\Delta)} \left[\frac{1}{E_0'-E_0+\Delta'} + \frac{1}{E_0'-E_0} \right] + \frac{\Delta'}{(E_0'-E_0)(E_0'-E_0+\Delta')} \left[\frac{1}{E_0+\Delta} + \frac{1}{E_0} \right] \right\} (S-9T)^{1/2} , \tag{43}$$

where P', Q, E_0', and Δ' are the parameters of the Γ_{15}^c conduction band. They are related to the parameter B by

$$B = P'Q \left[\frac{1}{E_0'-E_0+\Delta'} + \frac{1}{E_0'-E_0} \right] . \tag{44}$$

The first term in Eq. (43) agrees with our a_3 term represented by Eq. (42) while the second term can only be obtained by using the seven-band model. This further assures the reliability of our result for the valence band.

V. CONCLUSION

We have extended the applicability of our previous model to derive the energy wave-vector expansion for any **k·p** matrix of any size. We then applied this extended model to the 8×8 **k·p** matrix representing the band structure of zinc-blende-type semiconductors. We gave complete nonperturbative general expressions for the third-order terms of the valence band. These terms can now be used to study many interesting nonlinear[24] phenomena in a comprehensive way.

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[1] N. E. Christensen and M. Cardona, Solid State Commun. **49**, 491 (1984).
[2] U. Rossler, Solid State Commun. **49**, 943 (1984).
[3] M. Braun and U. Rossler, J. Phys. C **18**, 3365 (1985).
[4] M. Cardona, N. E. Christensen, and G. Fasol, Phys. Rev. B **38**, 1806 (1988).
[5] U. Ekenberg, Phys. Rev. B **40**, 7714 (1989).
[6] T. Ruf and M. Cardona, Phys. Rev. B **41**, 10 747 (1990).
[7] L. A. Cury and J. C. Portal, Phys. Rev. B **44**, 6224 (1991).
[8] H. J. Drouhin and J. Peretti, Phys. Rev. B **44**, 7993 (1991).
[9] M. I. Diakonov and V. I. Perel, in *Optical Orientation,* edited by V. M. Agranovich and A. A. Maradudin (North-Holland, Amsterdam, 1984), p. 11.
[10] G. E. Pikus and A. N. Titkov, in Ref. 9, p. 73.
[11] A. T. Gerelenko, B. A. Marushchak, and A. N. Titkov, Izv. Akad. Nauk SSSR Ser. Fiz. **50**, 290 (1986).
[12] W. Kauschke, N. Mestres, and M. Cardona, Phys. Rev. B **35**, 3843 (1987).
[13] M. A. Alekseev, V. D. Dymnikov, D. N. Mirlin, I. I. Reshina, and V. F. Sapega, Fiz. Tverd. Tela (Leningrad) **28**, 793 (1986)[Sov. Phys. Solid State **28**, 441 (1986)].
[14] Y. F. Chen, M. Dobrowolska, J. K. Furdyna, and S. Rodriguez, Phys. Rev. B **32**, 890 (1985).
[15] M. Cardona, N. E. Christensen, M. Dobrowolska, J. K. Furdyna, and S. Rodriguez, Solid State Commun. **60**, 171 (1986).
[16] H. Riechert, S. F. Alvarado, A. N. Titkov, and V. I. Safarov, Phys. Rev. Lett. **52**, 2297 (1984).
[17] M. Cardona, V. A. Maruschak, and A. N. Titkov, Solid State Commun. **50**, 701 (1984).
[18] S. S. Montasser, Phys. Rev. B **42**, 7513 (1990).
[19] E. O. Kane, in *Semiconductors and Semimetals,* edited by R. K.Willardson and A. C. Beer (Academic, New York, 1966), Vol. 1, p. 75.
[20] W. Fawcett, Proc. Phys. Soc. London **85**, 931 (1965).
[21] H.-R. Trebin, R. Rossler, and Ranvaud, Phys. Rev. B **20**, 686 (1979).
[22] G. Dresselhaus, Phys. Rev. **100**, 580 (1955).
[23] J. M. Luttinger, Phys. Rev. **102**, 1030 (1955).
[24] P. A. Wolff and G. A. Pearson, Phys. Rev. Lett. **17**, 1015 (1966).