SPIN-ORBIT INTERACTION IN SEMICONDUCTORS: CRITICAL ANALYSIS, DETAILS AND TEST CASES

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1. INTRODUCTION

In the work published almost ten years ago Chelikowsky and Cohen [1] suggested formula* for pseudopotential spin-orbit matrix elements. This formula has been intensively used for energy band calculations of elementary semiconductors and semiconductor compounds. Generalizing Bloom-Bergstresser's formula [2], which followed from modified Weisz's formula [3], the authors of the work [1] have given it in the form from which it is not easy to repeat their results. In some of the recent papers [4, 5], spin-orbit interaction influence has been estimated on the basis of that or similar formula. We are of the opinion that it is worth to give precise expression for pseudopotential spin-orbit interaction matrix elements.

2. SPIN-ORBIT INTERACTION

The formula for the pseudopotential spin-orbit interaction matrix elements for semiconductor compounds with zinc-blende cubic structure, which follows from Bloom-Bergstresser's work [2], can be written in the form:

$$< \vec{k}_i, \nu \,|W_{SO}|\, \vec{k}_j, \nu' > = \frac{\vec{k}_i \times \vec{k}_j}{k_i k_j} \cdot \vec{\sigma}_{\nu\nu'} \left[\lambda^A \sin (\vec{k}_i - \vec{k}_j) \vec{\tau} - i \lambda^S \cos (\vec{k}_i - \vec{k}_j) \vec{\tau}\right], \qquad (1)$$

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* Formula (13) in [1]

where

$$\lambda^S = \frac{\lambda_1 + \lambda_2}{2} \quad \text{and} \quad \lambda^A = \frac{\lambda_1 - \lambda_2}{2}, \tag{2}$$

are the symmetric and antisymmetric contributions to the spin-orbit Hamiltonian, $\vec{\sigma}$ is the Pauli spin operator, ν and ν' are spin indices. Vector product $\vec{k}_i \times \vec{k}_j$ in (1) is given in $(\frac{2\pi}{a})^2$ units, where a is lattice constant. All other wave vectors are taken in atomic units. Further $\vec{k}$ will denote the point from the first Brilioiun zone (BZ), $\vec{k}_i = \vec{k} + \vec{g}_i$, $\vec{k}_j = \vec{k} + \vec{g}_j$ and $\vec{g}_i$, $\vec{g}_j$ are reciprocal lattice vectors. The sine and cosine terms in (1) are appropriate for the geometrical structure factor of this lattice and $\vec{\tau} = \frac{a}{8}$ (111)

The λ_1 and λ_2 are contibutions of the first and second element in the mentioned binary compounds:

$$\lambda_1 = \mu B^1_{nl}(k_i)\, B^1_{nl}(k_j) \tag{3}$$

$$\lambda_2 = \alpha \mu B^2_{nl}(k_i)\, B^2_{nl}(k_j), \tag{4}$$

where μ is an adjustable parameter (in Ryd) and α is constrained such that the ratio of spin-orbit contribution for the atoms in binary compounds is the same as the spin-orbit splitting ratio for free atoms [6].

We include only contributions from the outermost p-core states. Contributions from inner core states or d-core states can be neglected [7].

$B^i_{nl}(k)$ is defined by

$$B^i_{nl}(k) = C \int_0^\infty j_l(kr)\, R^i_{nl}(r)\, r^2 dr, \tag{5}$$

where $R^i_{nl}(r)$ is the radial part of the core wave function, i denotes the element of binary compound ($i = 1, 2$), j_l is a spherical Bessel function, while C is the normalization constant defined so that

$$\lim_{k \to 0} k^{-l} B^i_{nl}(k) = 1 \tag{6}$$

Integrals defined in formulas (5) and (6) were solved numerically in [1] on the basis of tabulated data for radial part of atomic wave functions given in Herman-Skillman book [6]. However, these integrals can be solved analytically [8] on the basis of radial part of the core wave function obtained by the Roothaan-Hartree-Fock method [9]:

$$R_{nl}(r) = \sum_{p=1}^{N_g} c_{nlp}\, \chi_{lp}, \tag{7}$$

where N_g denotes the number of basis functions (Slater-type orbitals) having the form:

$$\chi_{lp} = [(2\,n_{lp})!]^{-1/2}\,(2\,\xi_{lp})^{n_{lp}+1/2}\,r^{n_{lp}-1}\,e^{-\xi_{lp} r} \tag{8}$$

The parameters c_{nlp}, n_{lp}, ξ_{lp} and number N_g for each atom are given in [9, 10]. In that way we obtained the analytic expression for integral (5)**

$$B_{nl}(k) = C\frac{k^l\sqrt{\pi}}{2^{l+1}}\sum_{p=1}^{N_g} c_{nlp}\,[(2n_{lp})!]^{-1/2}\,(2\,\xi_{lp})^{n_{lp}+1/2}\,\cdot$$

$$\cdot\frac{\Gamma(l+n_{lp}+2)}{\sqrt{(\xi_{lp}^2+k^2)}^{\,l+n_{lp}+2}\cdot\Gamma(l+\frac{3}{2})}\cdot F\left(\frac{n_{lp}+l+2}{2};\ \frac{l-n_{lp}}{2};\ l+\frac{3}{2};\ \frac{k^2}{\xi_{lp}^2+k^2}\right), \tag{9}$$

where F is hypergeometric function and Γ is Gamma function. The constant C is defined by the following relation:

$$C^{-1} = \frac{\sqrt{\pi}}{2^{\,l+1}}\sum_{p=1}^{N_g} c_{nlp}\cdot[(2n_{lp})!]^{-1/2}\,(2\,\xi_{lp})^{n_{lp}+\frac{1}{2}}\ \frac{\Gamma(l+n_{lp}+2)}{\xi_{lp}^{\,l+n_{lp}+2}\cdot\Gamma(l+3/2)} \tag{10}$$

3. DISCUSSION OF THE RESULTS

Nonlocal pseudopotential of Chelikowsky and Cohen has been tested for Si and GaP. In the case of these semiconductors the effect of spin-orbit splitting in respective energy levels can be neglected. We repeated results from [1]. In order to get these results we have to take:

1. d-well radius, which is not given in [1], has the same value for both components in the compound. That value is $\frac{a\sqrt{3}}{8}$ and was obtained by means of „touching spheres" approximation.

2. Matrix elements of the nonlocal pseudopotential were not included in perturbation terms.

3. In Brust-Löwdin's perturbation scheme, the same formula for diagonal and non-diagonal matrix elements in truncated secular equation had been used. The value of parameter $\bar{E}$ is $\bar{E} = 2\ (\frac{2\pi}{a})^2$ (see (25) in [11]).

4. According to the authors statement in [1] the solutions of the secular equation with satisfactory convergence was obtained for Löwdins parameters N ≈ 50 and L ≈ 100, where N is order of truncated and L is order of total secular equation. For example, we were able to repeat the results for energy levels in the point Γ from first BZ using N = 59 and L = 113 for GaP and N = 59 and L = 146 for Si.

** Let us note that the formulas (15), (17) and (18) from Ref. [8], have some mistakes which are corrected here. Appropriate corrections were also made in respective computer program SPINORB. New modified version of this program will be published.

The results for other semiconductors are given in columns HS and RHF in Tab. I. They are obtained by means of N = 59, L = 113 in the point Γ and N = 75, L = 146 in the points X and L. Chelikowsky-Cohen's results are given in the column CC. Results in the column HS in the same Table were obtained on the basis of numerical solutions of integrals (5). The data for radial wave functions from [6] were linearly interpolated. The

Table I.

Eigenvalues (eV) at Γ, X and L for indicated semiconductors. The column CC is taken from Ref. 1. The column HS is obtained by numerical solution and the column RHF by analytical solution of integrals (5), respectively.

	α – Sn				InAs			InSb		
	CC	HS	RHF		CC	HS	RHF	CC	HS	RHF
Γ_6^v	0.	0.	0.	Γ_6^v	0.	0.	0.	0.	0.	0.
Γ_7^v	10.54	10.56	10.54	Γ_7^v	12.26	12.27	12.27	10.89	10.88	10.90
Γ_7^c	10.92	10.92	10.92	Γ_8^c	12.69	12.70	12.69	11.71	11.73	11.71
Γ_8^v	11.34	11.34	11.34	Γ_6^c	13.06	13.07	13.07	11.96	11.96	11.96
Γ_6^c	13.42	13.44	13.43	Γ_7^c	17.08	17.08	17.09	14.87	14.88	14.89
Γ_8^c	14.00	13.99	14.00	Γ_8^c	17.32	17.32	17.32	15.30	15.31	15.30
				X_6^v	2.49	2.49	2.49	2.51	2.51	2.51
X_5^v	3.46	3.47	3.47	X_6^v	6.05	6.06	6.06	5.28	5.28	5.29
				X_6^v	10.22	10.20	10.20	9.26	9.24	9.25
X_5^v	8.59	8.57	8.57	X_7^v	10.32	10.31	10.30	9.47	9.46	9.45
				X_6^c	14.97	14.94	14.94	13.42	13.40	13.40
X_5^c	12.24	12.22	12.22	X_7^c	15.35	15.32	15.32	13.54	13.52	13.52
L_6^v	1.9	1.9	1.9	L_6^v	1.77	1.76	1.76	1.76	1.75	1.75
L_6^v	4.74	4.73	4.73	L_6^v	6.46	6.45	6.45	5.79	5.78	5.78
L_6^v	9.66	9.65	9.65	L_6^v	11.43	11.42	11.42	10.27	10.25	10.26
$L_{4,5}^v$	10.14	10.12	10.13	$L_{4,5}^v$	11.69	11.68	11.67	10.75	10.75	10.74
L_6^c	11.48	11.47	11.46	L_6^c	14.22	14.19	14.19	12.74	12.73	12.73
L_6^c	14.82	14.82	14.82	L_6^c	18.11	18.11	18.11	16.01	16.01	16.01
$L_{4,5}^c$	15.11	15.09	15.10	$L_{4,5}^c$	18.24	18.22	18.22	16.24	16.23	16.23

Table I. (continued)

	InP			GaSb			CdTe		
	CC	HS	RHF	CC	HS	RHF	CC	HS	RHF
Γ_6^v	0.	0.	0.	0.	0.	0.	0.	0.	0.
Γ_7^v	11.21	11.21	11.20	11.24	11.27	11.24	10.18	10.19	10.19
Γ_8^v	11.42	11.41	11.42	12.00	11.99	12.00	11.07	11.07	11.07
Γ_6^c	12.92	12.93	12.93	12.86	18.86	12.86	12.66	12.66	12.66
Γ_7^c	16.06	16.06	16.03	15.44	15.46	15.43	16.43	16.39	16.39
Γ_8^c	16.34	16.32	16.35	15.77	15.76	15.77	16.68	16.70	16.71
X_6^v	2.51	2.52	2.52	2.67	2.68	2.68	1.95	1.94	1.94
X_6^v	5.41	5.29	5.29	5.24	5.24	5.24	6.02	6.02	6.02
X_6^v	9.33	9.11	9.10	9.39	9.39	9.38	9.09	9.08	9.08
X_7^v	9.36	9.13	9.14	9.63	9.60	9.60	9.47	9.40	9.40
X_6^c	13.86	13.83	13.83	13.72	13.71	13.71	14.55	14.51	14.51
X_7^c	14.39	14.34	14.34	13.79	13.77	13.77	15.02	15.02	15.02
L_6^v	1.75	1.73	1.73	1.83	1.82	1.82	1.43	1.42	1.42
L_6^v	5.58	5.58	5.58	5.75	5.74	5.74	6.34	6.30	6.30
L_6^v	10.33	10.32	10.32	10.55	10.56	10.54	9.89	9.87	9.87
$L_{4,5}^v$	10.48	10.47	10.48	11.00	10.98	10.99	10.42	10.39	10.40
L_6^c	13.61	13.59	13.59	13.22	13.20	13.20	13.89	13.88	13.88
L_6^c	17.00	16.97	16.96	16.43	16.43	16.42	17.25	17.22	17.22
$L_{4,5}^c$	17.12	17.07	17.08	16.59	16.57	16.58	17.42	17.40	17.41

column RHF is obtained using analytical formulae (9) and (10). The spin-orbit parameter μ was adjusted in order to get respective experimental difference $\Gamma_8^v - \Gamma_7^v$ (as in the work [1]). The values of μ, together with more precise values of a obtained on the basis of recent data from [12], are given in Table II.

Let us emphasize some of the results emerging from the columns CC and HS of the Tab. I. Maximum difference is not greater than 0.02 eV for α – Sn, 0.03 eV for InAs, 0.03 eV for GaSb, and 0.02 eV for InSb. In the case CdTe appropriate difference is 0.04 eV, except for the level X_7^v where the difference is 0.07 eV. For some levels of InP

Table II.

The parameters μ and a used in this work. Data for μ in HS column are taken from [1], while the data for a in the same column are from [6]. The values for a in RHF column were obtained using the data from [12]. For the parameter μ in the same column explanation is given in the text.

	a– Sn		InAs		InSb		InP.		GaSb		CdTe	
	HS	RHF	HS	RHF	HS	RHF	HS	RHF	HS	RHF	HS	RHF
μ	0.00225	0.00261	0.0012	0.00125	0.0018	0.00185	0.0020	0.0025	0.0011	0.0012	0.00137	0.0015
a	–	–	0.7953	0.7663	1.2803	1.2871	0.1595	0.1381	2.2166	2.3144	1.6418	1.6548

maximum difference is of the order of 0.05 eV. The exceptions are X_6^V and X_7^V where the differencies are of the order ~ 0.1 – 0.2 eV. Here we want to say that these differencies were not influenced by spin-orbit splittings. All differencies, with the exception of emphasized X_7^V for CdTe, X_6^V and X_7^V for InP levels, are less or equal to the experimental errors (~ 0.05 eV). The cause of this discrepancy is not known to us.

We think that we excluded numerical errors which can emerge from the solutions of the integrals (5). The results were stable on the second decimale place when we applied different interpolation schemes, grid with 441 points generated in [6] for radial wave functions and double precision.

We are of the opinion that our results for X_7^V level of CdTe, X_6^V, X_7^V level of InP and other levels of Tab. I are correct. Almost the same results are obtained in the column RHF, on the basis of analytical solutions of integrals (5).

Let us stress once more that the choice of radial wave functions does not influence the band structure of semiconductors. The differencies between energy levels in the columns HS and RHF are not greater than 0.01 eV. This difference is little greater for Γ_7^C level of InP and Γ_7^C, Γ_8^C levels of CdTe.

Using the radial wave functions in the analytical form for arbitrary point in BZ we need less computer time (approximately by a factor two). This is important for the density of states calculations with spin-orbit interaction included.

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