

## Manipulation of the spin-orbit coupling using the Dirac equation for spin-dependent potentials

H. Ebert, H. Freyer, and M. Deng

*Institut für Physik. Chemie, Universität München, Theresienstrasse 37, D-80333 München, Germany*

(Received 27 May 1997)

A scheme is presented that allows one to decompose the spin-orbit coupling operator into two parts within calculations based on the Dirac equation for spin-dependent potentials. The first term lifts energetic degeneracies but leaves the spin as a good quantum number, while the second term causes hybridization of states with a different spin character. To investigate the importance of these terms and of the mechanism connected to them a number of model calculations for the dispersion relation, the spin-orbit-induced orbital magnetic moment, and the magneto-optical Kerr effect in several transition metal systems have been performed by retaining just one of them. In all cases studied it was found that the first term is by far the most important source for spin-orbit-induced phenomena. [S0163-1829(97)01340-4]

### I. INTRODUCTION

Recently there has been much interest in phenomena that are caused by the interplay of magnetism and spin-orbit interaction. Some examples of these are the magnetocrystalline anisotropy,<sup>1</sup> galvanomagnetic effects,<sup>2</sup> and the magnetic dichroism observed in any kind of spectroscopy of magnetic solids.<sup>3</sup> In most cases corresponding theoretical investigations are based on a perturbational or variational treatment of spin-orbit coupling when calculating the underlying electronic structure (for an overview see Ref. 4). However, during the past ten years several alternate band structure methods have been developed that are based on the solution of the Dirac equation for a spin-dependent potential, and that treat this way spin-orbit interaction and magnetism on the same footing. In a previous paper<sup>4</sup> (referred to in the following as paper I) it was demonstrated that even when starting with this sophisticated approach it is possible to identify the spin-orbit coupling individually in a set of approximate radial Dirac equations. This allows one to perform model calculations with the strength of the spin-orbit coupling manipulated—just as it can be done within a perturbational approach. Corresponding investigations have been done recently on the influence of the spin-orbit coupling strength on the orbital magnetic moment in alloys,<sup>4</sup> galvanomagnetic properties of disordered alloys,<sup>5</sup> the magneto-optical Kerr effect,<sup>4</sup> and the magnetic dichroism in x-ray absorption.<sup>6</sup> In the following it is demonstrated that a similar procedure as used before can be applied to split the spin-orbit coupling term into a part that breaks the orbital degeneracy but leaves the spin as a good quantum number and a second one that causes hybridization of the two spin subsystems. As will be shown below by several quite different applications corresponding investigations on the relative importance give a deeper insight into the origin of the above mentioned phenomena. In addition the results presented supply a justification for the use of much simpler calculation schemes that account for spin-orbit coupling in an approximate way when calculating the electronic structure of magnetic solids.

### II. DERIVATION OF APPROXIMATE RADIAL DIFFERENTIAL EQUATIONS

The starting point of our derivation is the Dirac Hamiltonian

$$\mathcal{H}_D = \frac{c}{i} \boldsymbol{\alpha} \cdot \nabla + \frac{1}{2} (\beta - I) + V(\mathbf{r}), \quad (1)$$

for the single site problem, i.e., an isolated potential well. The quantities  $\alpha_i$  and  $\beta$  are the standard Dirac matrices.<sup>7</sup> The potential  $V(\mathbf{r})$  is defined in the framework of the relativistic counterpart of nonrelativistic spin density functional theory<sup>8,9</sup> and consists of the Hartree term  $V_H(\mathbf{r})$  together with the spin averaged and spin-dependent part,  $\bar{V}_{xc}(\mathbf{r})$  and  $V_{spin}(\mathbf{r})$ , respectively, of the exchange-correlation potential:

$$V(\mathbf{r}) = V_H(\mathbf{r}) + \bar{V}_{xc}(\mathbf{r}) + V_{spin}(\mathbf{r}). \quad (2)$$

Without loss of generality one may assume the magnetization to point along the  $z$  axis leading for the spin-dependent part to

$$V_{spin}(\mathbf{r}) = \beta \sigma_z \frac{\partial E_{xc}}{\partial m(\mathbf{r})} = \beta \sigma_z B(\mathbf{r}), \quad (3)$$

with  $m(\mathbf{r})$  the spin magnetization density. To solve the single site Dirac equation corresponding to the above Hamiltonian one makes the ansatz for the four-component wave function<sup>10</sup>

$$\Psi(\mathbf{r}, E) = \sum_{\Lambda} \psi_{\Lambda}(\mathbf{r}, E) = \sum_{\Lambda} \begin{pmatrix} g_{\Lambda}(r, E) \chi_{\Lambda}(\hat{\mathbf{r}}) \\ if_{\Lambda}(r, E) \chi_{-\Lambda}(\hat{\mathbf{r}}) \end{pmatrix}, \quad (4)$$

where  $g_{\Lambda}$  and  $f_{\Lambda}$  are the major and minor radial wave functions. The functions  $\chi_{\Lambda}(\hat{\mathbf{r}})$  are the conventional spin-angular functions,<sup>7</sup>

$$\chi_{\Lambda}(\hat{\mathbf{r}}) = \sum_{m_s = \pm 1/2} C \left( \ell \frac{1}{2} j; \mu - m_s, m_s \right) Y_{\ell}^{\mu - m_s}(\hat{\mathbf{r}}) \chi_{m_s}, \quad (5)$$

with the Clebsch-Gordan coefficients  $C(\ell \frac{1}{2} j; \mu - m_s, m_s)$ , the complex spherical harmonics  $Y_{\ell}^{\mu - m_s}(\hat{\mathbf{r}})$ , and the Pauli spin functions  $\chi_{m_s}$ . Finally, the indices  $\Lambda$  and  $-\Lambda$  stand for  $(\kappa, \mu)$  and  $(-\kappa, \mu)$ , respectively, with  $\kappa$  and  $\mu$  the spin-orbit and magnetic quantum numbers.

Inserting the above ansatz into the Dirac equation leads to a set of an infinite number of coupled differential equations for wave functions with the same magnetic quantum number  $\mu$  and parity, i.e.,  $\Delta l = 0, 2, 4, \dots$ . Fortunately, in praxis this coupling can be restricted to  $\Delta l = 0$ .<sup>10</sup> For that reason, one is left with couplings of the type  $p_{1/2, \mu} - p_{3/2, \mu}$ ,  $d_{3/2, \mu} - d_{5/2, \mu}$ , and so on. By eliminating the minor component in the resulting first order differential equations, a second order differential equation for the major component has been obtained in paper I that is still exact and shows a term that can be identified with the spin-orbit coupling. The further strategy in that paper was to neglect the minor component, i.e., to switch to a two component formalism. This allowed us to scale the strength of the spin-orbit coupling in an arbitrary way with the resulting differential equation still formulated and solved using the conventional relativistic  $\Lambda$  representation.

Instead of manipulating the second order differential equation for the major component a corresponding wave equation in spherical coordinates is introduced here first for the two-component wave function  $\Phi(\mathbf{r}, E)$ :

$$\left[ -\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{\hat{K}^2}{r^2} - S_{\Lambda} T + S_{\Lambda} B \sigma_z + \frac{S'_{\Lambda}}{S_{\Lambda}} \left( \frac{d}{dr} - \frac{1}{r} - \frac{\hat{K} - 1}{r} \right) \right] \Phi(\mathbf{r}, E) = 0. \quad (6)$$

Here,  $\hat{K} = \boldsymbol{\sigma} \cdot \mathbf{l} + 1$  is the spin-orbit coupling operator<sup>7</sup> and the abbreviations

$$T = E - V, \quad (7)$$

$$S_{\Lambda} = \frac{E - V}{c^2} + 1 + \frac{B}{c^2} \langle \chi_{-\Lambda} | \sigma_z | \chi_{-\Lambda} \rangle \quad (8)$$

have been used, where  $S_{\Lambda}$  would be identical to 1 in the nonrelativistic limit which is obtained for  $c \rightarrow \infty$ .

For the wave function  $\Phi(\mathbf{r}, E)$  the ansatz,

$$\Phi(\mathbf{r}, E) = \sum_{\Lambda} \phi_{\Lambda}(\mathbf{r}, E) = \sum_{\Lambda} g_{\Lambda}(r, E) \chi_{\Lambda}(\hat{\mathbf{r}}), \quad (9)$$

is made in accordance with the adopted  $\Lambda$  representation. Inserting this ansatz into the wave equation (6) leads to the following second order radial differential equation:

$$P''_{\Lambda} = \frac{l(l+1)}{r^2} P_{\Lambda} - S_{\Lambda} T P_{\Lambda} + S_{\Lambda} \sum_{\Lambda'} B_{\Lambda \Lambda'} P_{\Lambda'} + \frac{S'_{\Lambda}}{S_{\Lambda}} \left[ \frac{d}{dr} - \frac{1}{r} \right] P_{\Lambda} + \frac{S'_{\Lambda}}{S_{\Lambda}} \frac{1}{r} \sum_{\Lambda'} \xi_{\Lambda \Lambda'} P_{\Lambda'}, \quad (10)$$

with  $P_{\Lambda} = r g_{\Lambda}$ . Here the spin-orbit coupling operator  $\hat{K}$  has been replaced using the operator

$$\hat{\xi} = \hat{K} - 1 = \boldsymbol{\sigma} \cdot \mathbf{l}, \quad (11)$$

with the corresponding angular matrix elements  $\xi_{\Lambda \Lambda'}$ . Inserting their proper values

$$\xi_{\Lambda \Lambda'} = \langle \chi_{\Lambda} | \hat{K} - 1 | \chi_{\Lambda'} \rangle = (-\kappa - 1) \delta_{\Lambda \Lambda'}, \quad (12)$$

the above-mentioned exact second order differential equation for the major component is recovered [see Eq. (13) in paper I].

Instead of allowing us only to manipulate the strength of the spin-orbit coupling Eq. (10) also allows us to modify the form of the spin-orbit coupling operator. For this purpose,  $\hat{\xi}$  is split according to

$$\hat{\xi} = \boldsymbol{\sigma} \cdot \mathbf{l} = \sigma_z l_z + (\sigma_x l_x + \sigma_y l_y) = \hat{\xi}_{zz} + \hat{\xi}_{xy} \quad (13)$$

into two parts. The first term,  $\hat{\xi}_{zz}$ , gives rise only to a splitting of levels with a different quantum numbers  $m_l$ . Because no mixing of states with a different spin character is introduced that way,  $m_s$  is left as a good quantum number. In contrast to this the second term,  $\hat{\xi}_{xy}$ , gives rise to a hybridization of different spin states while no obvious splitting of  $m_l$  levels is caused by it. Because the two parts of  $\hat{\xi}$  have quite different consequences it is interesting to investigate their effect separately by replacing  $\hat{\xi}$  in Eq. (10) either by  $\hat{\xi}_{zz}$  or by  $\hat{\xi}_{xy}$ . The corresponding angular matrix elements to be inserted are

$$\langle \chi_{\Lambda} | \hat{\xi}_{zz} | \chi_{\Lambda'} \rangle = \delta_{l l'} \delta_{\mu \mu'} \begin{cases} -\mu \sqrt{1 - \left( \frac{2\mu}{2l+1} \right)^2} & \text{for } \kappa \neq \kappa' \\ -S_{\kappa} \frac{2\mu^2}{2l+1} - \frac{1}{2} & \text{for } \kappa = \kappa' \end{cases} \quad (14)$$

$$\langle \chi_{\Lambda} | \hat{\xi}_{xy} | \chi_{\Lambda'} \rangle = \delta_{l l'} \delta_{\mu \mu'} \begin{cases} +\mu \sqrt{1 - \left( \frac{2\mu}{2l+1} \right)^2} & \text{for } \kappa \neq \kappa' \\ -\kappa + S_{\kappa} \frac{2\mu^2}{2l+1} - \frac{1}{2} & \text{for } \kappa = \kappa', \end{cases} \quad (15)$$

with  $S_{\kappa} = \kappa / |\kappa|$ . A solution of the resulting second order differential equation for the two different cases can be achieved by introducing the auxiliary function

$$Q_{\Lambda} = \left[ P'_{\Lambda} + \frac{\kappa}{r} P_{\Lambda} \right] \frac{1}{S_{\Lambda}}. \quad (16)$$

This leads to the following sets of coupled first order differential equations:

$$P'_{\Lambda} = -\frac{\kappa}{r} P_{\Lambda} + S_{\Lambda} Q_{\Lambda}, \quad (17)$$

$$Q'_\Lambda = \frac{\kappa}{r} Q_\Lambda - TP_\Lambda + \sum_{\Lambda'} B_{\Lambda\Lambda'} P_\Lambda - \frac{S'_\Lambda}{S_\Lambda} \frac{1}{r} \left[ (\kappa+1)P_\Lambda + \sum_{\Lambda'} \xi_{\Lambda\Lambda'}^\lambda P_{\Lambda'} \right], \quad (18)$$

with  $\xi_{\Lambda\Lambda'}^\lambda = \langle \chi_\Lambda | \hat{\xi}_{zz} | \chi_{\Lambda'} \rangle$  or  $\xi_{\Lambda\Lambda'}^\lambda = \langle \chi_\Lambda | \hat{\xi}_{xy} | \chi_{\Lambda'} \rangle$ , respectively.

These final equations differ from the original coupled radial Dirac equations for the major and minor components, where one has  $P_\Lambda = rg_\Lambda$  and  $Q_\Lambda = crf_\Lambda$ , only because of the last term in Eq. (18). Implementing these model equations is therefore extremely simple. Apart from this additional term nearly no further modifications have to be done for a band structure program that is based on the fully relativistic Hamiltonian in Eq. (1). However, one again has to note that  $Q_\Lambda$  in Eq. (18) has not the meaning of a minor component of a four-component wave function. For that reason for the calculation of any physical quantity only forms of the corresponding matrix elements may be used that do not involve any combinations of the major and the minor component wave functions, as, for example, the electric dipole matrix element in its  $\boldsymbol{\alpha} \cdot \mathbf{A}$  form (see paper I).

### III. APPLICATIONS

The scheme described above has been implemented and combined with the spin-polarized relativistic (SPR) version of a linear-muffin-tin-orbital<sup>11</sup> (LMTO) as well as a Korringa-Kohn-Rostoker<sup>12</sup> (KKR) band structure program. This means that it has been used within a conventional  $\vec{k}$ -space variational method and a method based on multiple scattering theory, respectively. Results of corresponding applications are presented and discussed in the following.

#### A. Dispersion relation of fcc-Ni

To demonstrate the effect of the various parts of the spin-orbit coupling the dispersion relation  $E(\vec{k})$  of Ni has been calculated in a proper relativistic way; i.e., using the full Dirac equation as well as using the scheme presented above keeping for  $\hat{\xi}$  only its part  $\hat{\xi}_{zz}$  or  $\hat{\xi}_{xy}$ , respectively. Figure 1 shows corresponding results for the magnetization  $\vec{M}$  along the [001] axis and the wave-vector  $\vec{k}$  along the [100] axis. As has been mentioned above, spin-orbit coupling gives rise to the lifting of degeneracies (e.g., at A and B in Fig. 1, top) and causes hybridization or mixing of bands (e.g., at C, D, E, and F) that simply cross within a nonrelativistic treatment. In addition the expectation value of  $\langle \Psi_{j\vec{k}} | \sigma_z | \Psi_{j\vec{k}} \rangle$  is not restricted to  $\pm 1$  (see, e.g., Refs. 13,14), i.e., spin is no more a good quantum number. However, remarkable deviations from the values  $\pm 1$  occur only in the region where bands cross, if spin-orbit coupling is neglected. For that reason it is justified to attach the labels  $\downarrow$  and  $\uparrow$  to the bands to indicate their dominant spin character for a certain range of  $\vec{k}$ .

Keeping only the  $\hat{\xi}_{zz}$  part of the spin-orbit interaction the most important consequence is that now all states have pure spin character that cannot change if one goes along a certain

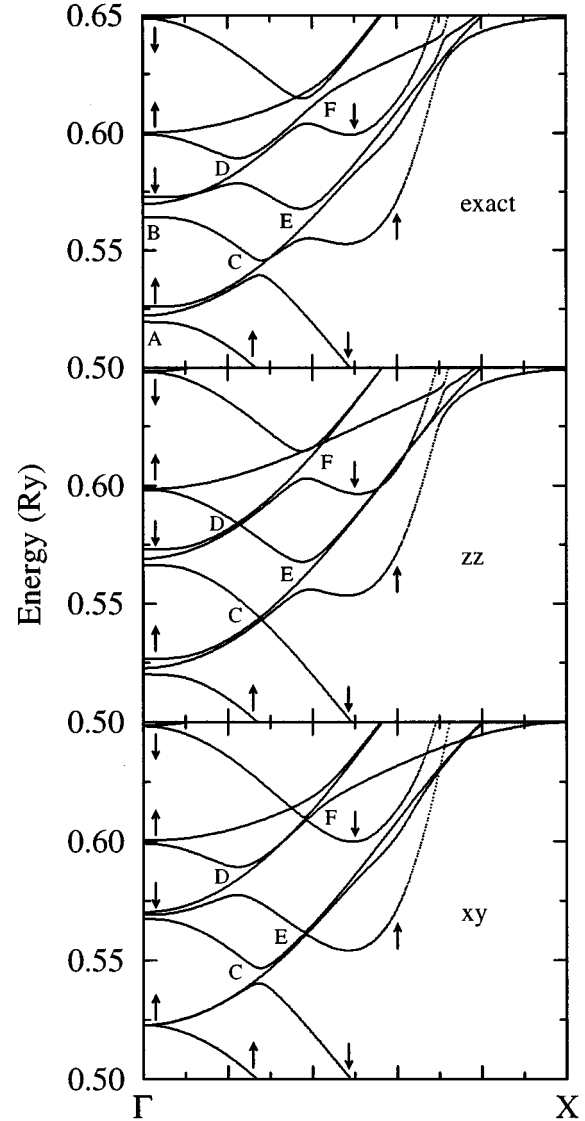


FIG. 1. Dispersion relation  $E(\vec{k})$  of fcc-Ni for the magnetization  $\vec{M}$  and the wave vector  $\vec{k}$  along the [001] and [100] axes, respectively. The panels show from top to the bottom results based on the full Dirac equation and those obtained keeping the  $zz$  and  $xy$  terms in Eq. (13).

band. However, this does not rule out the hybridization of bands induced by  $\hat{\xi}_{zz}$ . As one can see from the middle panel of Fig. 1 hybridization takes place at E and F. On the other hand, no hybridization is found at C and D, where now bands of different spin character cross. Furthermore one notes that the splitting of the bands, e.g., at A, B, E, and F caused by the  $\hat{\xi}_{zz}$  part is quite comparable to that due to the full spin-orbit interaction.

Concerning the hybridization, the situation is more or less opposite to the situation for  $\hat{\xi}_{zz}$ , if the  $\hat{\xi}_{xy}$  part is used. The lower panel of Fig. 1 demonstrates that there is now a pronounced hybridization of bands of different spin character (C and D)—just as for the full spin-orbit interaction. While hybridization is also present at E and F it is much less pronounced than for  $\hat{\xi}_{zz}$ . Surprisingly, the splitting of the bands

TABLE I. Spin-orbit-induced orbital magnetic moments (in  $\mu_B$ ) of pure Fe, Co, and Ni, respectively, obtained without any manipulation (exact) and keeping the  $zz$  and  $xy$  terms, respectively, in Eq. (13).

	bcc-Fe	fcc-Co	fcc-Ni
Exact	0.0534	0.0749	0.0505
$zz$	0.0536	0.0756	0.0504
$xy$	-0.0005	-0.0008	-0.0002

caused by  $\hat{\xi}_{xy}$ , while being in general smaller than for  $\hat{\xi}_{zz}$ , is still quite appreciable. In spite of this, both parts have a rather different importance for many spin-orbit-induced properties, as will be demonstrated below.

Obviously, the scheme presented above allows us to investigate quantitatively the consequences of the two parts of the spin-orbit interaction and to trace back the origin of the observed hybridization in a simple and straightforward way. Of course, this could also be achieved within an analytical approach treating the various parts of the spin-orbit coupling as a perturbation for a spin-split band structure and studying the symmetry for these situations.

### B. Spin-orbit-induced orbital magnetic moments

One of the most prominent spin-orbit-induced magnetic property is the orbital magnetic moment  $\mu_{orb}$  in transition metals. Using the tabulated experimental values<sup>15</sup> this amounts to 10% of the total magnetic moment for Co and Ni and to 5% for Fe. For these elements corresponding theoretical values for  $\mu_{orb}$  are given in Table I. These data have been obtained applying the standard expression<sup>12</sup>

$$\mu_{orb} \approx \langle \hat{I}_z \rangle \mu_B, \quad (19)$$

with  $\hat{I}_z$  the  $z$  component of the orbital angular momentum operator. The calculations have been performed using the SPR-KKR method ignoring the so-called orbital polarization mechanism<sup>16</sup> which leads to an enhancement of the spin-orbit-induced orbital magnetic moment.

Comparing the results for the three sets of calculations one notes that the two different manipulations of the spin-orbit coupling considered here have very different consequences. Using  $\hat{\xi}_{zz}$  gives in all cases results for  $\mu_{orb}$  that are only slightly higher than for the full spin-orbit coupling term  $\hat{\xi}$ . Using  $\hat{\xi}_{xy}$  instead leads to very small moments that are found to be of opposite sign. Adding the moments obtained for  $\hat{\xi}_{zz}$  and  $\hat{\xi}_{xy}$ , respectively, the original value is nearly recovered. Obviously the  $xy$  part of the complete spin-orbit coupling operator has the effect to slightly reduce the orbital magnetic moment that is induced by the  $zz$  part by lifting the degeneracy of the  $m_l$  sublevels.

While for the pure elements the effect of manipulating the spin-orbit coupling is quite straightforward, the situation can get rather complex for alloys or compounds. Table II summarizes results obtained for bcc-Fe<sub>0.8</sub>Co<sub>0.2</sub> for which the magnetic moments and the spin-orbit coupling strength of both components are quite similar. As one can see, keeping for Fe just  $\hat{\xi}_{zz}$  has also some effect for  $\mu_{orb}$  of Co. This

TABLE II. As for Table I, but for Fe and Co in the disordered alloy bcc-Fe<sub>0.8</sub>Co<sub>0.2</sub>. The labels Fe, Co, and both in column one indicate for which components the corresponding spin-orbit coupling term is manipulated.

	Fe	Co
Exact	0.0564	0.0899
$zz$ (Fe)	0.0564	0.0906
$xy$ (Fe)	0.0066	0.0690
$zz$ (Co)	0.0566	0.0903
$xy$ (Co)	0.0492	0.0201
$zz$ (both)	0.0565	0.0907
$xy$ (both)	0.0005	0.0009

means that the distortion is transferred via hybridization to the Co site. On the other hand, using  $\hat{\xi}_{zz}$  for the Co sites has only little impact on  $\mu_{orb}$  of Fe ( $\mu_{orb}^{Fe}$ ) because of the high Fe concentration. For the same reason, keeping  $\hat{\xi}_{xy}$  for Fe reduces  $\mu_{orb}^{Co}$  by 23% while there is only a reduction of 13% for  $\mu_{orb}^{Fe}$  if  $\hat{\xi}_{xy}$  is used for Co. Finally, if both components are manipulated the same way, the effect is quite similar to the situation of the pure system. This means if  $\hat{\xi}$  is replaced by  $\hat{\xi}_{zz}$  throughout only a small change is induced while the orbital magnetic moments nearly vanish if only  $\hat{\xi}_{xy}$  is kept.

In contrast to Fe<sub>0.8</sub>Co<sub>0.2</sub> the magnetic moments as well as the spin-orbit coupling strength differ by an order of magnitude for the two components of fcc-Co<sub>0.5</sub>Pt<sub>0.5</sub>. In addition their concentration has been chosen to be the same. In line with the previous results the consequence of replacing the spin-orbit coupling operator  $\hat{\xi}$  for any site or both sites by  $\hat{\xi}_{zz}$  has only a small consequence for the orbital magnetic moments. Replacing it by  $\hat{\xi}_{xy}$  for both components  $\mu_{orb}$  is nearly vanishing for Co and Pt (last line of Table III). However, if  $\hat{\xi}$  is replaced by  $\hat{\xi}_{xy}$  on just one site there is a rather unexpected consequence. If  $\hat{\xi}_{xy}$  is used for Co,  $\mu_{orb}^{Pt}$  increases slightly. Manipulating the Pt sites that way, the on-site moment  $\mu_{orb}^{Pt}$  is reduced to less than 9% while  $\mu_{orb}^{Co}$  increases by 55% at the same time. On the other hand, a reduction to  $-0.048\mu_B$  is found when  $\hat{\xi}_{xy}$  replaces  $\hat{\xi}$  for the Co sites. Therefore one has to conclude that, the weaker that the spin-orbit coupling strength is effectively on the Co site compared to that on the Pt site, the smaller  $\mu_{orb}^{Co}$  is. This is in line with

TABLE III. As for Table II, but for Co and Pt in the disordered alloy fcc-Co<sub>0.5</sub>Pt<sub>0.5</sub>.

	Co	Pt
Exact	0.0847	0.0592
$zz$ (Co)	0.0851	0.0591
$xy$ (Co)	-0.0480	0.0650
$zz$ (Pt)	0.0853	0.0594
$xy$ (Pt)	0.1321	0.0050
$zz$ (both)	0.0859	0.0596
$xy$ (both)	-0.0015	0.0005

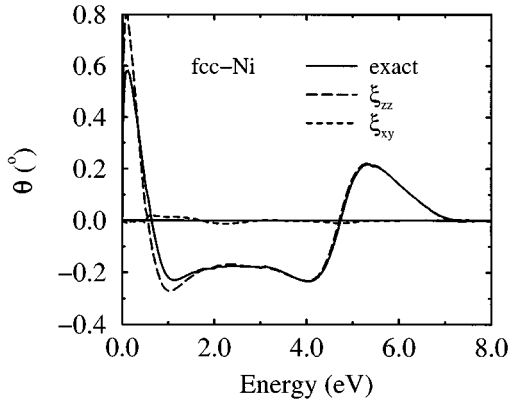


FIG. 2. Magneto-optical Kerr rotation angle  $\theta_K$  for fcc-Ni: obtained without any manipulation (exact) and keeping the  $zz$  and  $xy$  terms, respectively.

the previous finding that  $\mu_{\text{orb}}^{\text{Co}}$  monotonously decreases and gets negative when going from pure Co to the Pt-rich side of  $\text{Co}_x\text{Pt}_{1-x}$ .<sup>17</sup>

### C. Magneto-optical Kerr effect

Another interesting spin-orbit-induced phenomenon is the magneto-optical Kerr effect. For technical applications of this effect the most important quantity is the Kerr-rotation angle  $\theta_K$ . For the so-called polar geometry<sup>18</sup>  $\theta_K$  gives the rotation of the polarization vector that is observed when linearly polarized light is reflected from a sample that is magnetized parallel or antiparallel to the light beam. For photon energies higher than 1–2 eV the optical properties—and with these the Kerr-rotation—are determined by  $\vec{k}$ -conserving electronic interband transitions.<sup>18</sup>

Looking upon spin-orbit coupling as a perturbation for a spin-polarized band structure, Erskine and Stern<sup>19</sup> proposed three distinct possible sources of the Kerr rotation for that situation: (i) lifting of degeneracies of energy levels, (ii) hybridization of states with different spin character, and (iii) spin-flip transitions due to spin-orbit coupling. Point (iii) arises because spin-orbit interaction gives rise to a correction term to the nonrelativistic form of the electric dipole matrix element.<sup>20</sup> The importance of this correction has been investigated in the past by several authors.<sup>20–24</sup> For FePt, for which it should be quite pronounced because of the high atomic number of Pt, Guo and Ebert<sup>24</sup> found changes in the matrix elements in the order of 1%. The scheme presented above now allows us to perform model calculations aiming to investigate the role of points (i) and (ii) in addition. Results of corresponding calculations of the Kerr-rotation angle  $\theta_K$  of fcc-Ni performed using the SPR-LMTO method are shown in Fig. 2. As one can see, the spectrum obtained on the basis of  $\hat{\xi}_{zz}$  alone is astonishingly close to the original spectrum. Only for small photon energies do pronounced differences in the absolute magnitude of the rotation angle occur. Keeping on the other hand only the term  $\hat{\xi}_{xy}$ , a very small rotation is found. Quite similar to the situation for  $\mu_{\text{orb}}$  of Fe, Co, and Ni, the rotation spectra based on  $\hat{\xi}_{zz}$  and  $\hat{\xi}_{xy}$  alone add up to the proper spectrum.

Investigating the Kerr-rotation spectrum of an ordered compound is somewhat more complex than dealing with a

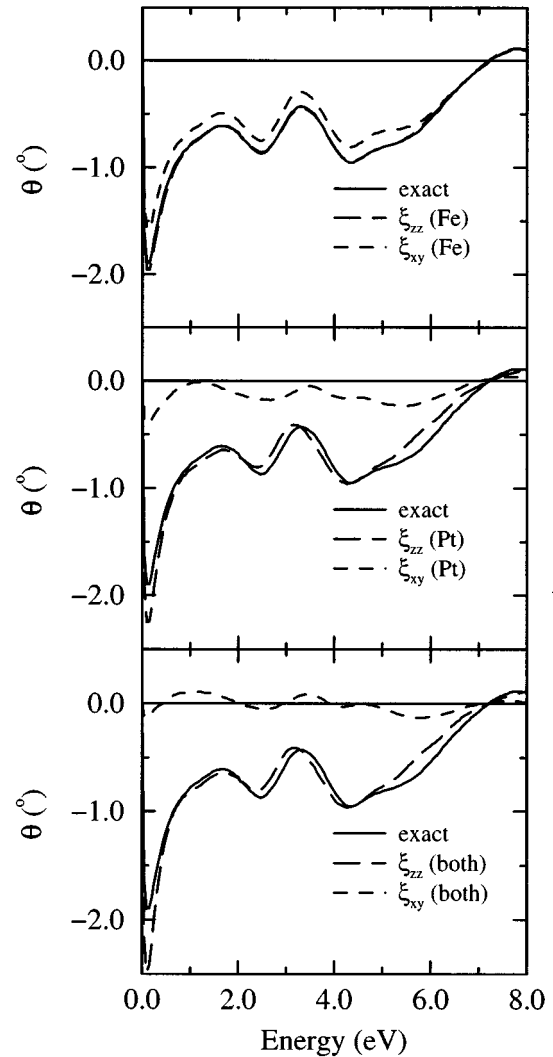


FIG. 3. As for Fig. 1 but for the compound FePt. The various panels show from top to bottom results obtained manipulating only the Fe, the Pt, and all sites, respectively.

pure element, because the various components can contribute to a different extent. For FePt, for example, the spin-orbit interaction on the Fe site is obviously of minor importance, as can be seen in Fig. 3. Replacing the full spin-orbit interaction operator  $\hat{\xi}$  by  $\hat{\xi}_{zz}$  on the Fe site has a rather small impact on the spectrum (see top of Fig. 3). If only  $\hat{\xi}_{xy}$  is kept on the other hand, the magnitude of the rotation is reduced by an appreciable amount. Nevertheless, manipulating the spin-orbit coupling on the Pt site has a much stronger impact (see middle of Fig. 3). Keeping just  $\hat{\xi}_{zz}$  not only changes the amplitude of  $\theta_K$  but also affects the position of minima and maxima of the spectrum. If only  $\hat{\xi}_{xy}$  is kept for the Pt sites, the rotation is strongly diminished demonstrating that the Kerr-rotation spectrum of FePt is—at least concerning the spin-orbit coupling—dominated by Pt. This is once more reflected by the results obtained for both sites manipulated. Keeping just  $\hat{\xi}_{zz}$  one gets nearly the same spectrum as obtained by replacing  $\hat{\xi}$  only on the Pt site. If  $\hat{\xi}_{xy}$  substitutes  $\hat{\xi}$  on all sites the resulting rotation is again quite small and oscillating.

The investigations mentioned above concerning point (iii) together with the results presented here clearly demonstrate that among the variations sources of the Kerr rotation discussed by Erskine and Stern<sup>19</sup> the mechanism (i), i.e., the lifting of degeneracies by  $\hat{\xi}_{zz}$  is by far the most important one. This means that the hybridization of states of different spin character plays only a minor role not only for the pure 3d-transition metals but also for compounds containing heavy elements.

#### D. Approximate treatment of spin-orbit coupling within a conventional spin-polarized band structure calculation

The results presented above demonstrate that one gets quite reliable or at least semiquantitative results for spin-orbit induced properties if only  $\hat{\xi}_{zz}$  is accounted for—even if the studied system contains heavy elements. Because the term  $\hat{\xi}_{zz}$  leaves the spin quantum number  $m_s$  as a good quantum number it is extremely simple to be incorporated within a non- or scalar-relativistic band structure program for spin-dependent potentials. In fact this approximate treatment of spin-orbit coupling has been adopted in the past by various authors without giving a detailed justification for this. For example, Hübner<sup>25</sup> used this approximation in discussing the nonlinear magneto-optical Kerr effect. Akai<sup>26</sup> has performed calculations for  $\mu_{orb}$  of Fe, Co, and Ni getting results very similar to those given in Table I. Also his calculations for the magnetic circular x-ray dichroism at the  $K$  edge of Fe and Ni in disordered  $\text{Fe}_x\text{Ni}_{1-x}$  alloys<sup>26</sup> gave results in accordance with corresponding fully relativistic calculation.<sup>27</sup>

The only complication that arises if  $\hat{\xi}_{zz}$  is incorporated in a conventional band structure program is the fact that one has to solve radial differential equations for each set of  $(l, m_l)$  quantum numbers. However, there is no coupling of different partial waves introduced by  $\hat{\xi}_{zz}$ . Because the size of the Hamilton and overlap matrices occurring within a variational band structure scheme or of the scattering matrices occurring within multiple scattering theory, respectively, does not change due to  $\hat{\xi}_{zz}$ , the numerical effort increases only slightly compared to a calculation without  $\hat{\xi}_{zz}$ . Accounting for the full spin-orbit coupling instead would double the size of the matrices and for that reason increases

the computing time of the band structure part by a factor of 4 (not 8 because the system is assumed to be spin polarized).

In spite of the simple form of  $\hat{\xi}_{zz}$  one has to note that it nevertheless breaks the symmetry of the system—otherwise the various phenomena discussed above would not occur. This means that, for example, the magnetocrystalline anisotropy energy can also be calculated on the basis of this simplified spin-orbit coupling term. Because of the simple form of  $\hat{\xi}_{zz}$  the magnetocrystalline anisotropy can be investigated within a modified non- or scalar-relativistic band structure calculation in a similar way as the noncollinear spin magnetism is treated.<sup>28,29</sup>

#### IV. CONCLUSIONS

A scheme has been presented that allows—starting from the Dirac equation for a spin-dependent potential—to split the spin-orbit interaction into a part lifting the energetic degeneracy and a second one introducing the hybridization of states with a different spin character. This was shown explicitly by calculations of the dispersion relations of Ni for which one of these parts was suppressed. For the spin-orbit-induced phenomena investigated here—orbital magnetic moment and Kerr rotation—it turned out that the first mechanism is by far the dominating one. This result obviously supplies a deeper insight into the physical origin of these phenomena. In addition it gives justification for the use of an approximate treatment of spin-orbit interaction by accounting just for the first part that is diagonal with respect to spin. For the properties studied here one should get at least semiquantitative agreement with the proper fully relativistic results that way—even for systems containing heavy elements. However, this does not necessarily apply also for other spin-orbit-induced properties. For galvanomagnetic properties, for example, one might expect that spin mixing plays quite an important role. Corresponding investigations to confirm this expectation are on the way at the moment.

#### ACKNOWLEDGMENTS

This work was funded by the DFG (Deutsche Forschungsgemeinschaft) within the program *Theorie relativistischer Effekte in der Chemie und Physik schwerer Elemente*.

<sup>1</sup>B. Újfalussy, L. Szunyogh, P. Bruno, and P. Weinberger, Phys. Rev. Lett. **77**, 1805 (1996).

<sup>2</sup>J. Banhart and H. Ebert, Europhys. Lett. **32**, 517 (1995).

<sup>3</sup>*Spin-orbit Influenced Spectroscopies of Magnetic Solids*, edited by H. Ebert and G. Schütz, Lecture Notes in Physics Vol. 466 (Springer-Verlag, Heidelberg, 1996).

<sup>4</sup>H. Ebert, H. Freyer, A. Vernes, and G.-Y. Guo, Phys. Rev. B **53**, 7721 (1996).

<sup>5</sup>J. Banhart, A. Vernes, and H. Ebert, Solid State Commun. **98**, 129 (1996).

<sup>6</sup>H. Ebert, V. Popescu, and D. Ahlers, J. Phys. IV **7**, C2-131 (1997).

<sup>7</sup>M. E. Rose, *Relativistic Electron Theory* (Wiley, New York, 1961).

<sup>8</sup>A. H. MacDonald and S. H. Vosko, J. Phys. C **12**, 2977 (1979).

<sup>9</sup>M. V. Ramana and A. K. Rajagopal, J. Phys. C **12**, L845 (1979).

<sup>10</sup>R. Feder, F. Rosicky, and B. Ackermann, Z. Phys. B **52**, 31 (1983).

<sup>11</sup>H. Ebert, Phys. Rev. B **38**, 9390 (1988).

<sup>12</sup>H. Ebert, P. Strange, and B. L. Gyorffy, J. Phys. F **18**, L135 (1988).

<sup>13</sup>B. Ackermann, R. Feder, and E. Tamura, J. Phys. F **14**, L173 (1984).

<sup>14</sup>R. Richter and H. Eschrig, Solid State Commun. **72**, 263 (1989).

<sup>15</sup>M. B. Stearns, in *Magnetic Properties of 3d, 4d and 5d Elements, Alloys and Compounds*, edited by K.-H. Hellwege and O. Madelung, Landolt-Börnstein, New Series, Group III, Vol. 19, Pt. a (Springer, Berlin, 1987).

- <sup>16</sup>H. Ebert and M. Battocletti, *Solid State Commun.* **98**, 785 (1996).
- <sup>17</sup>H. Ebert and H. Akai, *Hyperfine Interact.* **78**, 361 (1993).
- <sup>18</sup>H. Ebert, *Rep. Prog. Phys.* **59**, 1665 (1996).
- <sup>19</sup>J. L. Erskine and E. A. Stern, *Phys. Rev. Lett.* **30**, 1329 (1973).
- <sup>20</sup>C. S. Wang and J. Callaway, *Phys. Rev. B* **9**, 4897 (1974).
- <sup>21</sup>D. K. Misemer, *J. Appl. Phys.* **61**, 3355 (1987).
- <sup>22</sup>D. K. Misemer, *J. Magn. Magn. Mater.* **72**, 267 (1988).
- <sup>23</sup>G. H. O. Daalderop, F. M. Mueller, R. C. Albers, and A. M. Boring, *J. Appl. Phys. Lett.* **52**, 1636 (1988).
- <sup>24</sup>G. Y. Guo and H. Ebert, *Phys. Rev. B* **51**, 12 633 (1995).
- <sup>25</sup>W. Hübner, *Phys. Rev. B* **42**, 11 553 (1990).
- <sup>26</sup>H. Akai (private communication).
- <sup>27</sup>H. Ebert and H. Akai, in *Application of Multiple Scattering Theory to Material Science*, edited by W. H. Butler, P. H. Dederichs, A. Gonis, and R. Weaver, MRS Symposia Proceedings No. 253 (Materials Research Society, Pittsburgh, 1992), p. 329.
- <sup>28</sup>L. M. Sandratskii, *Phys. Status Solidi B* **135**, 167 (1986).
- <sup>29</sup>L. M. Sandratskii, *Solid State Commun.* **75**, 527 (1990).