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

H. Ebert, H. Freyer, and A. Vernes
Institute for Physical Chemistry, University of Munich, Theresienstrasse 37, D-80333 München, Germany

G.-Y. Guo
Daresbury Laboratory, Daresbury, Warrington WA4 4AD, United Kingdom
(Received 11 August 1995)

A scheme is presented that allows us to manipulate the spin-orbit coupling in calculations based on the Dirac equation for spin-dependent potentials. To demonstrate its application, the spin and orbital magnetic moments for the disordered alloy $Fe_{0.20}Ni_{0.80}$ as well as the Kerr rotation angle θ_K of pure Ni have been calculated as a function of the spin-orbit coupling strength. While the spin moment changes only slightly, the orbital moment as well as the Kerr rotation angle θ_K increase almost linearly with the spin-orbit coupling strength.

INTRODUCTION

The importance of relativistic effects for the electronic structure of solids was realized decades ago. Accordingly various authors have generalized most methods of band-structure calculation already in the 1960s [APW,[1] OPW,[2] KKR,[3,4] and ASW (Ref. 5)].

To avoid the increased technical and numerical requirements connected with these fully relativistic versions based on the Dirac equation, a number of appropriate schemes have been proposed that aimed to account at least for the relativistic mass enhancement and the Darwin term.[6–12] The spin-orbit coupling (SOC), on the other hand, was either completely neglected or incorporated in an averaged way. By getting rid of the symmetry-breaking effect of the SOC, these so-called scalar relativistic schemes keep spin as a good quantum number. This feature allows one to perform spin polarized calculations for spin-magnetic systems accounting at least for some of the relativistic effects in a very simple way, i.e., by replacing just the subroutine to calculate the radial wave functions while leaving all other parts of the programs unchanged.

However, these scalar relativistic schemes obviously do not allow us to study phenomena in magnetic solids that are due to the symmetry breaking caused by the SOC. A conceptionally simple way to account for this demand is to deal with SOC as a perturbation in the variational step of a conventional band-structure scheme.[13–17] On the other hand, the technical problems of dealing with the Dirac equation for an isolated spin-dependent potential (single site problem) were solved by various authors in the beginning of the 1980s.[18–20] This development opened the way to derive corresponding spin polarized relativistic (SPR) generalizations of the various band-structure schemes [KKR,[19,21] LMTO,[22] and ASW (Ref. 23)] allowing us to deal with spin polarization and all relativistic effects on the same footing.

During the last years these SPR band-structure methods have been applied with great success to study a great variety of phenomena caused by SOC in magnetic solids (orbital hyperfine fields and magnetic moments,[24] magnetocrystalline anisotropy,[25] magnetic x-ray dichroism,[26] magneto-optical Kerr effect,[27] spontaneous magnetoresistance anisotropy, and anomalous Hall resistivity[28]). The results of these studies are in general very close to those obtained using a scalar relativistic band-structure scheme that accounts for SOC in the variational step. However, the great advantage of the SPR methods is that they are open to any new development in the field of density functional theory for magnetic systems. Furthermore the SPR-KKR method can be combined straightforwardly with the coherent potential approximation alloy theory (SPR-KKR-CPA) to deal with disordered alloys.[29,30]

The only real drawback of the SPR schemes is that it was not possible so far to study the relationship of any physical quantity and the SOC strength in a direct way. Using a variational scheme corresponding model calculations can be done very easily by scaling the SOC matrix element.[31,32] In a SPR-type calculation based on the Dirac equation this can be achieved only by varying the speed of light c. However, this way all relativistic effects are modified. An approximate scheme to circumvent this problem that requires only minor changes in the programs is presented in the following together with some applications to demonstrate its usefulness.

I. DERIVATION OF APPROXIMATE RADIAL DIFFERENTIAL EQUATIONS

To supply a basis for relativistic band-structure calculations for magnetic solids various authors[33,34] suggested an extension of nonrelativistic spin density functional theory by using the Dirac Hamiltonian

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

with the standard Dirac matrices α_i and β.[35] Here the potential $V(\mathbf{r})$ consists of the Hartree term $V_{\mathrm{H}}(\mathbf{r})$ and a contribution due to exchange and correlation splitted into a spin averaged and spin-dependent part

$$V(\mathbf{r}) = V_{\mathrm{H}}(\mathbf{r}) + \bar{V}_{\mathrm{xc}}(\mathbf{r}) + V_{\mathrm{spin}}(\mathbf{r}). \tag{2}$$

The spin-dependent part of the $V_{\mathrm{spin}}(\mathbf{r})$ behaves like a magnetic field that couples only to the spin of the electron. For

this reason it may be combined with a possibly present external magnetic field $\mathbf{B}_{\rm ext}(\mathbf{r})$ as part of the effective field $\mathbf{B}_{\rm eff}(\mathbf{r})$,

$$V_{\rm spin}(\mathbf{r})=\beta\boldsymbol{\sigma}\cdot\left[\mathbf{B}_{\rm ext}(\mathbf{r})+\frac{\partial E_{\rm xc}(\mathbf{r})}{\partial\mathbf{m}(\mathbf{r})}\right]=\beta\boldsymbol{\sigma}\cdot\mathbf{B}_{\rm eff}(\mathbf{r}). \quad (3)$$

To solve the Dirac equation for a solid the first step within almost any band-structure scheme is to solve this equation for a single isolated potential well (single site problem). In the following it is assumed that the potential terms occurring in Eq. (1) are spherically symmetric (muffin-tin or atomic sphere approximation), i.e., $V(\mathbf{r})=V(r)$ and $\mathbf{B}_{\rm eff}(\mathbf{r})=B_{\rm eff}(\mathbf{r})\hat{\mathbf{z}}$ with $V(r)$ standing in the following for the spin-independent part of the potential [see Eq. (3)].

A solution $\Psi(\mathbf{r},E)$ to the single site Dirac equation corresponding to the Hamiltonian in Eq. (1) can be constructed making the ansatz

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

Here Λ and $-\Lambda$ stand for (κ,μ) and $(-\kappa,\mu)$, respectively, with κ and μ the spin-orbit and magnetic quantum numbers.[35] To simplify the notation we omit for $\Psi(\mathbf{r},E)$, $\Psi_{\Lambda}(\mathbf{r},E)$, $g_{\Lambda}(r,E)$, and $f_{\Lambda}(r,E)$ in Eq. (4) and the following an additional index that numbers the various independent solutions to Eq. (1).[20] The functions $\chi_{\Lambda}(\hat{\mathbf{r}})$ that occur in Eq. (4) are the conventional spin angular functions[35]

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

with the Clebsch-Gordon coefficients $C(\ell\frac{1}{2}j;\mu-m_s,m_s)$, the complex spherical harmonics $Y_{\ell}^{m}(\hat{\mathbf{r}})$, and the Pauli spin functions χ_{m_s}.

The ansatz for $\Psi_{\Lambda}(\mathbf{r},E)$ in Eq. (4) results in the following coupled set of radial differential equations for the major and minor wave functions $g(r,E)$ and $f(r,E)$, respectively,[18–20]

$$P'_{\Lambda}=-\frac{\kappa}{r}P_{\Lambda}+\left[\frac{E-V}{c^2}+1\right]Q_{\Lambda}+\frac{B}{c^2}\sum_{\Lambda'}\langle\chi_{-\Lambda}|\sigma_3|\chi_{-\Lambda'}\rangle Q_{\Lambda'}, \quad (6)$$

$$Q'_{\Lambda}=\frac{\kappa}{r}Q_{\Lambda}-[E-V]P_{\Lambda}+B\sum_{\Lambda'}\langle\chi_{\Lambda}|\sigma_3|\chi_{\Lambda'}\rangle P_{\Lambda'}, \quad (7)$$

with $P(r,E)=g(r,E)r$ and $Q(r,E)=cf(r,E)r$ suppressing the arguments r and E. In principle one has a coupling of an infinite number of partial waves $\Psi_{\Lambda}(\mathbf{r},E)$ having the same parity (i.e., $\Delta l=|l'-l|=0,2,4,\ldots$) and the same magnetic quantum numbers ($\Delta\mu=\mu'-\mu=0$), i.e., μ is a good quantum number. This general case has been studied by Ackermann[36] and recently by Jenkins and Strange in detail.[37] Fortunately, in practice it is sufficient to restrict the coupling to $\Delta l=0$ and $\Delta\mu=0$. Using the abbreviations

$$S_{\Lambda}=\frac{E-V}{c^2}+1+\frac{B}{c^2}\langle\chi_{-\Lambda}|\sigma_3|\chi_{-\Lambda}\rangle, \quad (8)$$

$$T=E-V, \quad (9)$$

and

$$B_{\Lambda\Lambda'}=B\langle\chi_{\Lambda}|\sigma_3|\chi_{\Lambda'}\rangle, \quad (10)$$

Eqs. (6) and (7) may be written as

$$P'_{\Lambda}=-\frac{\kappa}{r}P_{\Lambda}+S_{\Lambda}Q_{\Lambda}, \quad (11)$$

$$Q'_{\Lambda}=\frac{\kappa}{r}Q_{\Lambda}-TP_{\Lambda}+\sum_{\Lambda'}B_{\Lambda\Lambda'}P_{\Lambda'}, \quad (12)$$

where at most two partial waves $\Psi_{\Lambda}(\mathbf{r},E)$ are coupled (for $|\mu|<l$).

Obviously there is no term in Eqs. (11) and (12) that can unambiguously be identified with the SOC. However, this can be accomplished by inserting Eq. (11) into Eq. (12) leading to

$$P''_{\Lambda}=\frac{l(l+1)}{r^2}P_{\Lambda}-S_{\Lambda}TP_{\Lambda}+S_{\Lambda}\sum_{\Lambda'}B_{\Lambda\Lambda'}P_{\Lambda'}+\frac{S'_{\Lambda}}{S_{\Lambda}}\left[\frac{d}{dr}-\frac{1}{r}+\underbrace{\frac{\kappa+1}{r}}_{\rm SOC}\right]P_{\Lambda}. \quad (13)$$

For the paramagnetic case a corresponding second order differential equation for $Q_{\Lambda}(r,E)$ is obtained by inserting Eq. (12) into (11) with l and κ replaced by $\bar{l}$ and $-\kappa$, respectively.

Comparing Eq. (13) with the radial Schrödinger equation it can be seen that the last term on the right hand side has no nonrelativistic counterpart and it is the only term that depends on the SOC quantum number κ.[10]

To arrive at an approximate scheme that accounts for all relativistic effects and allows to manipulate the SOC strength we require that the corresponding wave function is determined by an equation identical in form to Eq. (13) with just the SOC term modified. For this purpose we drop the requirement that $\Psi(\mathbf{r},E)$ is a bispinor and instead of Eq. (4) we make the ansatz

$$\Psi(\mathbf{r},E)=\sum_{\Lambda}\phi_{\Lambda}(\mathbf{r},E)=\sum_{\Lambda}g_{\Lambda}(r,E)\chi_{\Lambda}(\hat{\mathbf{r}}), \quad (14)$$

i.e., we are still working in the Λ representation. The spin-angular functions $\chi_{\Lambda}(\hat{\mathbf{r}})$ [see Eq. (5)] are eigenfunctions of the spin-orbit operator $\hat{K}$,[35]

$$\hat{K}\chi_{\Lambda}(\hat{\mathbf{r}})=-\kappa\chi_{\Lambda}(\hat{\mathbf{r}}), \quad (15)$$

with

$$\hat{K}=1+\mathbf{s}\cdot\boldsymbol{l}, \quad (16)$$

where $\mathbf{s}$ and $\boldsymbol{l}$ are the spin and orbital angular momentum operators, respectively. If we manipulate the SOC strength by multiplying $\mathbf{s}\cdot\boldsymbol{l}$ with a scaling factor x, the functions $\chi_{\Lambda}(\hat{\mathbf{r}})$ are still eigenfunctions of the corresponding modified spin-orbit operator $\hat{K}_x$,

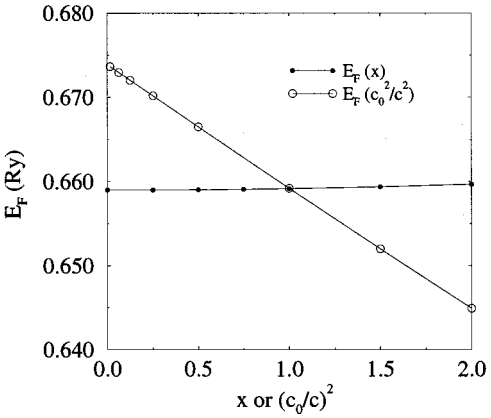

FIG. 1. Fermi energy E_F of $Fe_{0.20}Ni_{0.80}$ as a function of the scaling parameters x and $(c_0/c)^2$.

$$\hat{K}_x \chi_\Lambda(\hat{\mathbf{r}}) = -\kappa_x \chi_\Lambda(\hat{\mathbf{r}}), \tag{17}$$

where

$$\hat{K}_x = 1 + x\mathbf{s}\cdot\boldsymbol{l} \tag{18}$$

and

$$\kappa_x = -1 + x(1+\kappa). \tag{19}$$

For $x=1$ nothing changes at all, while for $x=0$ one gets $\kappa_x=-1$. This is just the value of the spin-orbit quantum number for s states where there is no SOC. Therefore, replacing κ in Eq. (13) by κ_x switches the SOC off for any partial wave if $x=0$ and reduces or increases the SOC strength else.

To solve the second order differential equation

$$P''_\Lambda = \frac{l(l+1)}{r^2} P_\Lambda - S_\Lambda T P_\Lambda + S_\Lambda \sum_{\Lambda'} B_{\Lambda\Lambda'} P_{\Lambda'} + \frac{S'_\Lambda}{S_\Lambda}\left[\frac{d}{dr} - \frac{1}{r} + \frac{\kappa_x + 1}{r}\right] P_\Lambda \tag{20}$$

for the wave functions $P_\Lambda(r,E)$ we introduce the auxiliary function $Q_\Lambda(r,E)$ by the definition

$$Q_\Lambda = \left[P'_\Lambda + \frac{\kappa_x}{r} P_\Lambda\right] \frac{1}{S_\Lambda}. \tag{21}$$

This allows us to derive a coupled set of first order differential equations which, after some simple transformations, are given by

$$P'_\Lambda = -\frac{\kappa_x}{r} P_\Lambda + S_\Lambda Q_\Lambda, \tag{22}$$

$$Q'_\Lambda = \frac{\kappa_x}{r} Q_\Lambda - T P_\Lambda + \sum_{\Lambda'} B_{\Lambda\Lambda'} P_{\Lambda'} + \frac{l(l+1) - \kappa_x(\kappa_x+1)}{r^2} \frac{1}{S_\Lambda} P_\Lambda. \tag{23}$$

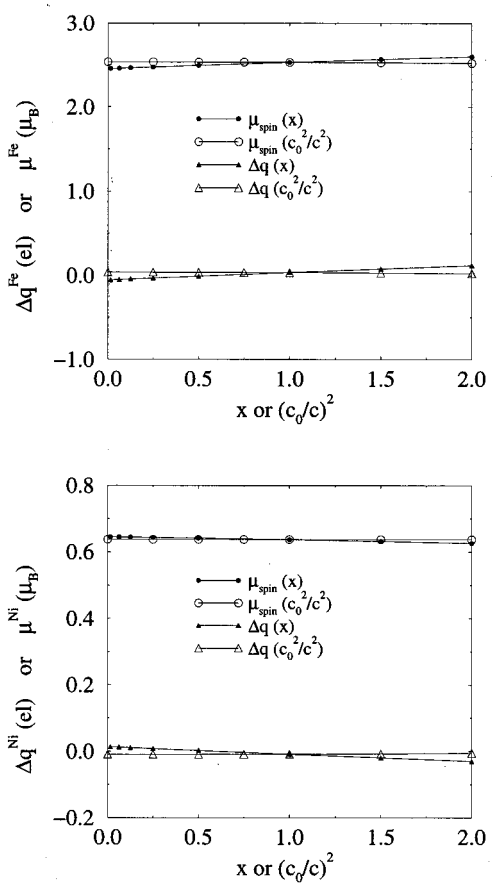

FIG. 2. Spin magnetic moment μ_{spin} and charge difference $\Delta q = q_{\text{atom}} - q_{\text{solid}}$ of Fe (top) and Ni (bottom) in $Fe_{0.20}Ni_{0.80}$ as a function of the scaling parameters x and $(c_0/c)^2$, with q_{atom} and q_{solid} the charge for the free atom and in the solid, respectively.

Apart from the last term in Eq. (23) these equations have the same form as the original Eqs. (11) and (12). Implementation of the above scheme therefore requires only minor modifications of the programs.

However, one has to keep in mind that $Q_\Lambda(r,E)$ defined by Eq. (21) has not the meaning of a minor component in a bispinor formalism. For this reason the boundary conditions which match the wave functions to the solutions outside the sphere boundary have to be specified through $P_\Lambda(r,E)$ alone.[22] To set up the corresponding single site t matrix $t_{\Lambda\Lambda'}(E)$ used within the KKR formalism one therefore has to replace the relativistic Wronskian (see Ref. 38) by its standard form $g_\Lambda(r,E) j'_l(r,E) - g'_\Lambda(r,E) j_l(r,E)$, where $j_l(r,E)$ is the spherical Bessel function. Furthermore one has to keep in mind that for the evaluation of the matrix elements of any operator it has to be transformed in such a way that no coupling of major and minor component occurs. This applies, for example, to the operator $\boldsymbol{\alpha}\cdot\mathbf{A}$ that describes the interaction of electrons with the vector potential $\mathbf{A}$. In this case, for example, the $\boldsymbol{\nabla}\cdot\mathbf{A}$ form of the matrix elements can be used.[27]

Finally, it should be noted that, in general, the results obtained from Eqs. (22) and (23) are expected to be close to those obtained if the approach of McLaren and Victoria would be used.[39] These authors start from the scalar-relativistic equations of Koelling and Harmon[8] and add the

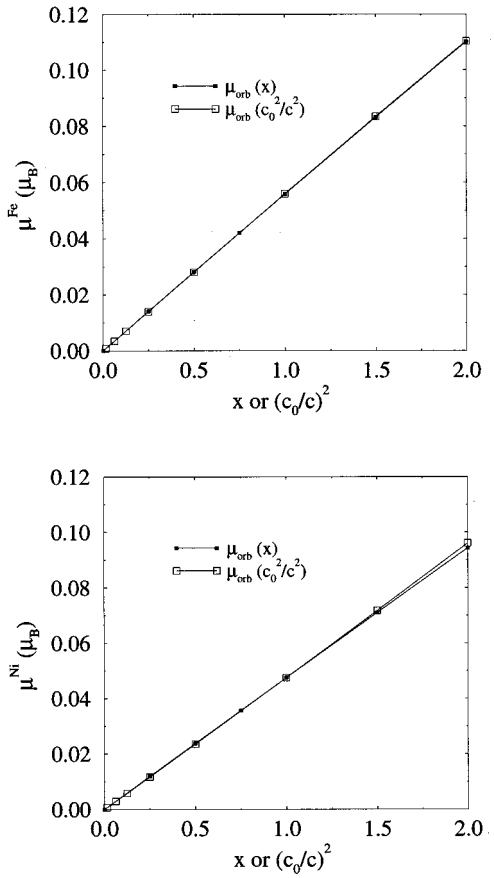

FIG. 3. Orbital magnetic moment μ_{orb} of Fe (top) and Ni (bottom) in $Fe_{0.20}Ni_{0.80}$ as a function of the scaling parameters x and $(c_0/c)^2$.

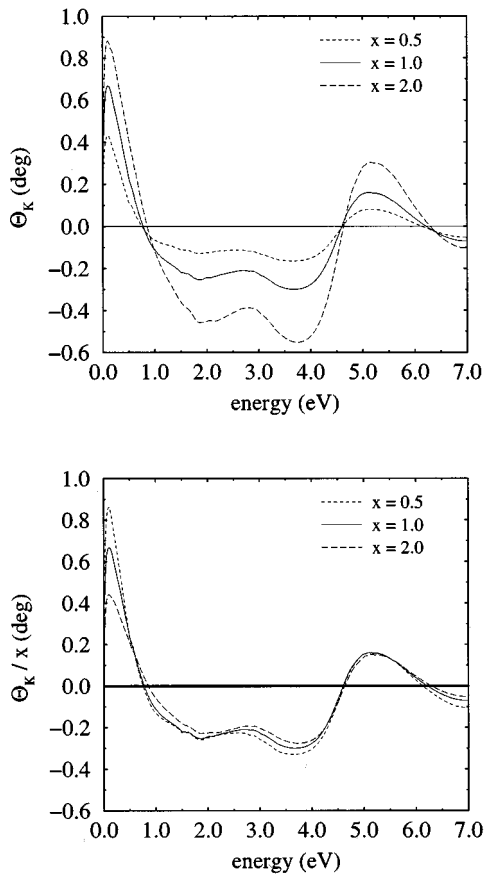

FIG. 4. Magneto-optical Kerr rotation angle θ_K of pure Ni as a function of the SOC strength scaling parameter x. The lower panel gives the normalized rotation spectra θ_K/x.

SOC term in its conventional form. Apart from working throughout within a (l,m_l,m_s) representation their approach ends up with a radial differential equation similar to Eq. (13).

II. APPLICATIONS

The scheme presented above has been implemented as part of a SPR-LMTO as well as a SPR-KKR program. Making use of the coherent potential approximation (CPA) alloy theory, the SPR-KKR method is applicable to disordered alloys in a rather straightforward way. In the following corresponding results for $Fe_{0.20}Ni_{0.80}$ are presented that have been obtained using a frozen potential stemming from a self-consistent scalar-relativistic calculation.

Figures 1–3 show the Fermi energy and the spin and orbital magnetic moments of Fe and Ni, respectively, for the SOC scaling parameter x varying from 0 to 2, i.e., from the nonrelativistic to a superrelativistic situation. In addition, results are presented that have been obtained by varying the speed of light to manipulate the impact of relativistic effects. Because the leading relativistic corrections to the Schrödinger equation are proportional to $1/c^2$, these data are plotted as a function of $(c_0/c)^2$ with c_0 the correct speed of light in vacuum.

As can be seen in Fig. 1, varying x, i.e., just the SOC, has only a very small influence on the Fermi energy E_F. This was to be expected from the fact that the SOC lifts degeneracies but leaves the center of gravity of the electronic bands unchanged. Similar calculations for $Co_{0.20}Pd_{0.80}$ (where the components of the alloy system strongly differ in their atomic numbers) show accordingly a larger impact on E_F. Increasing $(c_0/c)^2$ on the other hand causes, even for $Fe_{0.20}Ni_{0.80}$, the Fermi level to move to lower energies in a pronounced way. The reason for this is that, starting from the nonrelativistic limit, the mass velocity and Darwin terms, which act effectively as an attractive potential, are gradually switched on, thus moving all electronic states to lower energies. The changes of the Fermi level with x and $(c_0/c)^2$, respectively, are accompanied by corresponding changes in the spin magnetic moment μ_{spin}. Varying just the SOC via x has nearly no impact on μ_{spin}—only a small change for the both components can be observed. On the other hand $(c_0/c)^2$ strongly affects μ_{spin} due to the binding induced by the relativistic effects which is more pronounced for the s and p electrons than for the d electrons. As is demonstrated in Fig. 2, for the system studied here, the primary consequence of this is an internal charge rearrangement. This redistribution in turn is accompanied by a corresponding change in the spin magnetic moment because of dominating minority spin character at the Fermi energy.

Within a nonrelativistic description of electronic structure the orbital angular moment in a solid is quenched and the corresponding orbital magnetic moment μ_{orb} vanishes for that reason. SOC causes this quenching to be uncomplete

leading to a finite orbital magnetic moment.

As can be seen in Fig. 3, the orbital magnetic moment $\mu_{\rm orb}$ of Fe and Ni induced by SOC is nicely proportional to x as well as to $(c_0/c)^2$. Although in alloys where the difference in the atomic numbers of the components is higher than in case of $Fe_{0.20}Ni_{0.80}$, e.g., for $Co_{0.20}Pd_{0.80}$, the deviation from the linearity of $\mu_{\rm orb}(x)$ and also of $\mu_{\rm orb}(c_0^2/c^2)$ is more pronounced, of course.

As for $\mu_{\rm orb}$ also the magneto-optical Kerr rotation angle θ_K can be traced back to the symmetry breaking caused by SOC. The results for pure Ni obtained using the SPR-LMTO method demonstrate that again a nearly linear dependence of θ_K on the SOC strength is found (see Fig. 4, top). This result is in full accordance with the findings of Oppeneer *et al.*[31] From the ratio θ_K/x in Fig. 4 (bottom) it can be seen that deviations from proportionality occur primarily at low energies. Neglecting any contributions coming from the Drude term, as done here, this range of energy is related to electronic transitions in the vicinity of the Fermi energy E_F. With increasing photon energy $\hbar\omega$ more and more transitions involving states further away from E_F in energy contribute to the spectrum leading obviously to some canceling of the differences of the various normalized θ_K/x spectra.

Manipulation of the SOC of just one component of a compound can give valuable hints for the interpretation of its Kerr rotation spectrum. This has been demonstrated by the work of Sticht[32] and also recently by Oppeneer *et al.*[31] Using a tight-binding scheme corresponding calculations have recently been done for the magnetic x-ray dichroism (MXD) at the K edges of the pure elements Fe, Co, and Ni (Ref. 40) manipulating the SOC strength of the final valence p and d states separately. With the help of the above formalism this type of model calculation can also be done using a SPR band-structure method. For the $L_{2,3}$ edges of Co and Pt in the alloy $Co_{80}Pt_{20}$ no significant influence of SOC of one component on the spectrum of the other via hybridization could be found this way.[41] This is in some contrast to the Kerr rotation of compounds[42] and ensures that concerning the role of SOC the MXD is predominantly a site-specific phenomenon.

III. SUMMARY

A scheme has been presented to allow the direct manipulation of the SOC strength within relativistic band-structure calculations for magnetic systems leaving all other relativistic effects unaffected. Its application has been demonstrated by calculating the spin and orbital magnetic moments of Fe and Ni in the disordered alloy $Fe_{0.20}Ni_{0.80}$ as well as the Kerr rotation of pure Ni. As expected or found before, respectively, the orbital magnetic moment and the Kerr rotation varies nearly linearly with SOC strength. It is pointed out that corresponding model calculations of magneto-optical spectra in the visible or x-ray regime supply very helpful information supporting the interpretation of the — in general — very complex spectra.

ACKNOWLEDGMENTS

This work was funded by the DFG (Deutsche Forschungsgemeinschaft) within the programme *Theorie Relativistischer Effekte in der Chemie und Physik schwerer Elemente*. In addition it benefited from collaborations within the HCM-network on *Ab-initio (From Electronic Structure) Calculation of Complex Processes in Materials* (Contract No. ERBCHRXCT930369) and the programme *Relativistic Effects in Heavy-Element Chemistry and Physics (REHE)* of the European Science Foundation.

[1] T. L. Loucks, Phys. Rev. **139**, A1333 (1965).
[2] P. Soven, Phys. Rev. **137**, A1706 (1965).
[3] Y. Onodera and M. Okazaki, J. Phys. Soc. Jpn. **21**, 2400 (1966).
[4] S. Takada, Progr. Theor. Phys. Suppl. **36**, 224 (1966).
[5] T. Takeda, J. Phys. F **9**, 815 (1979).
[6] F. Rosicky and F. Mark, J. Phys. B **8**, 2581 (1975).
[7] F. Rosicky, P. Weinberger, and F. Mark, J. Phys. B **9**, 2971 (1976).
[8] D. D. Koelling and B. N. Harmon, J. Phys. C **10**, 3107 (1977).
[9] H. Gollisch and L. Fritsche, Phys. Status Solidi B **86**, 145 (1978).
[10] T. Takeda, Z. Phys. B **32**, 43 (1978).
[11] J. H. Wood and A. M. Boring, Phys. Rev. B **18**, 2701 (1978).
[12] H. L. Skriver, *The LMTO Method* (Springer, Berlin, 1983).
[13] J. Callaway and C. S. Wang, Phys. Rev. B **7**, 1096 (1973).
[14] O. K. Andersen, Phys. Rev. B **12**, 3060 (1975).
[15] M. S. S. Brooks and P. J. Kelly, Phys. Rev. Lett. **51**, 1708 (1983).
[16] J. Sticht and J. Kübler, Solid State Commun. **53**, 529 (1985).
[17] X.-F. Zhong, Y.-N. Xu, and W.-Y. Ching, Phys. Rev. B **41**, 10 545 (1990).
[18] S. Doniach and C. Sommers, in *Valence Fluctuations in Solids*, edited by L. M. Falicov, W. Hanke, and M. B. Maple (North-Holland, Amsterdam, 1981), p. 349.
[19] R. Feder, F. Rosicky, and B. Ackermann, Z. Phys. B **52**, 31 (1983).
[20] P. Strange, J. B. Staunton, and B. L. Gyorffy, J. Phys. C **17**, 3355 (1984).
[21] P. Strange, H. Ebert, J. B. Staunton, and B. L. Gyorffy, J. Phys. Condens. Matter **1**, 2959 (1989).
[22] H. Ebert, Phys. Rev. B **38**, 9390 (1988).
[23] B. C. H. Krutzen and F. Spingelkamp, J. Phys. Condens. Matter **1**, 8369 (1989).
[24] H. Ebert, P. Strange, and B. L. Gyorffy, J. Phys. F **18**, L135 (1988).
[25] P. Strange, J. B. Staunton, and H. Ebert, Europhys. Lett. **9**, 169 (1989).
[26] H. Ebert, P. Strange, and B. L. Gyorffy, J. Appl. Phys. **63**, 3055 (1988).
[27] G. Y. Guo and H. Ebert, Phys. Rev. B **50**, 10 377 (1994).
[28] H. Ebert and J. Banhart, Europhys. Lett. **32**, 517 (1995).
[29] H. Ebert, B. Drittler, and H. Akai, J. Magn. Magn. Mater. **104-107**, 733 (1992).
[30] H. Ebert and H. Akai, in *Application of Multiple Scattering Theory to Materials Science*, edited by W. H. Butler, P. H. Dederichs, A. Gonis, and R. L. Weaver, MRS Symposia Proceedings No. 253 (Materials Research Society, Pittsburgh, 1992), p. 329.

[31] P. M. Oppeneer, J. Sticht, T. Maurer, and J. Kübler, Z. Phys. B **88**, 309 (1992).
[32] D. Weller *et al.*, Phys. Rev. Lett. **69**, 2307 (1992).
[33] A. H. MacDonald and S. H. Vosko, J. Phys. C **12**, 2977 (1979).
[34] M. V. Ramana and A. K. Rajagopal, J. Phys. C **12**, L845 (1979).
[35] M. E. Rose, *Relativistic Electron Theory* (Wiley, New York, 1961).
[36] B. Ackermann, Ph.D. thesis, University of Duisburg, 1985.
[37] A. C. Jenkins and P. Strange, J. Phys. Condensed Matter **6**, 3499 (1994).
[38] H. Ebert and B. L. Gyorffy, J. Phys. F **18**, 451 (1988).
[39] J. M. MacLaren and R. H. Victora, J. Appl. Phys. **76**, 6069 (1994).
[40] J. Igarashi and K. Hirai, Phys. Rev. B **50**, 17 820 (1994).
[41] H. Ebert (unpublished).
[42] P. M. Oppeneer, V. N. Antonov, and T. Kraft (unpublished).