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1996 J. Phys.: Condens. Matter 8 10601

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J. Phys.: Condens. Matter **8** (1996) 10601–10608. Printed in the UK

Relativistic calculation of the electronic structure of antiferromagnetic chromium with a sinusoidal spin-density wave

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Received 19 June 1996, in final form 10 September 1996

Abstract. A simple method for calculating the electronic structure of antiferromagnetic chromium with a sinusoidal spin-density wave, based on the variational Ritz procedure, is suggested. The four-component Dirac wavefunctions, defined in a crystal without allowance for magnetic order, are chosen as basis functions. The calculations of the electronic spectrum of chromium performed for different types of spin-density wave polarization show that taking into account the relativistic effects results in a difference between the electronic structures of the longitudinal and transverse spin-density waves.

1. Introduction

In recent years, much research has been devoted to the electronic structure of antiferromagnetic (AF) chromium. The extensive literature on the subject has been reviewed in [1]. We shall dwell briefly on the main results of both experimental and theoretical investigations.

It has been found experimentally that, at temperatures below 312 K, chromium has AF order with a spin-density wave (SDW) incommensurate with the lattice constant. The wavevector $\boldsymbol{Q} = (2\pi/a)(1-\delta, 0, 0)$ (a is the lattice constant and $\delta \approx 0.05$) of the SDW is oriented in the direction of one of the cubic axes. As a consequence the unit cell contains about 40 chemically equivalent atoms with different magnitudes of the magnetic moment. The local magnetic moments are collinear and sinusoidally modulated with a maximum value $M = 0.59\mu_B$. Aside from the fundamental harmonic, higher harmonics ($3\boldsymbol{Q}, 5\boldsymbol{Q}$...) also occur. At a temperature of 118 K, the SDW polarization changes from longitudinal to transverse (the spin-flip phase transition).

It is clear that an *ab-initio* calculation of the ground state of AF Cr, based on actual experimental data on the magnetic structure, would be at the moment absolutely unfeasible. That is why most calculations are performed for a vector $\boldsymbol{Q} = (2\pi/a)(1, 0, 0)$. In this case, Cr has a CsCl unit cell. The local magnetic moments at different atoms are equal in magnitude but opposite in direction. Such an approach has been used, in particular, in [2–4], in which the electronic structure of Cr is calculated within the framework of spin-density functional theory. AF ordering is shown to cause a decrease in the density of states at the Fermi level due to the appearance of an AF gap, which results in a gain in total energy. The results obtained confirm Lomer's [5] supposition as to the role of the nesting character of the electronic and hole sheets of the Fermi surface of non-magnetic Cr in the formation of the AF state. Additional investigation of the structure of AF Cr Fermi

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surface and its pressure dependence has been reported in [4]. Our paper [6] is devoted to the study of the influence of relativistic effects on the electronic structure of chromium. The results of calculations demonstrate that the relativistic effects completely change the structure of the Cr electron spectrum, which leads to its anisotropy for directions identical in the non-relativistic approach.

A first-principles calculation of the total energy for a four-atom magnetic cell of Cr ($\boldsymbol{Q} = (2\pi/a)(0.5, 0, 0)$) has been carried out in [7]. The main result of the paper is the statement that for such a cell the ground state is not AF.

In a number of papers the parametrization of the electronic structure of non-magnetic Cr near the Fermi surface is used to give a qualitative description of the experimental data for the incommensurate spin-density wave (ISDW) of Cr and its alloys. So, in [8] the optical absorption in chromium with an ISDW was investigated in a one-dimensional two-band model, while in [9] the ISDW was studied using a two-band nesting model within the mean-field approximation.

Finally, in [10] the sinusoidal SDW was treated with a model *tight-binding* Hamiltonian whose parameters are assumed to be constant (except for the energy of d orbitals) and are calculated for paramagnetic Cr.

From the above it appears that a variety of approaches can be used to study the ground state of AF chromium with a SDW. Up to now, however, there have been no first-principles calculations of the electronic structure of chromium with a SDW, because these require huge computational efforts owing to the large dimension of dispersive matrices.

In the present paper we suggest a simple technique for calculating the electronic structure in the presence of a SDW, based on the variational Ritz procedure.

2. General formalism

In accordance with [11], the Dirac equation for a system with SDW can be written as

$$(\hat{H}_0 + \Delta V \hat{\Sigma})\Psi = E\Psi \tag{1}$$

where Ψ is a four-component spinor and $\hat{H}_0$ is the standard Dirac operator given by

$$\hat{H}_0 = c\hat{\alpha}\hat{\boldsymbol{p}} + mc^2\hat{\beta} + V\hat{I}. \tag{2}$$

Here

$$\hat{\alpha} = \begin{bmatrix} 0 & \sigma \\ \sigma & 0 \end{bmatrix} \qquad \hat{\beta} = \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix} \qquad \hat{\Sigma} = \begin{bmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{bmatrix} \tag{3}$$

$\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices and **I** is the unit matrix. We also assume the magnetic moment to be oriented in the Z direction.

Thus, the effective electron potential at site $\boldsymbol{R}_j$ consists of two terms: the site-independent average potential $V(\boldsymbol{r})$ and an addition $\Delta V_j(\boldsymbol{r})$ connected with spin polarization.

The variational Ritz procedure reduces the problem of solving (1) to solving the generalized eigenvalue problem

$$\sum_{n'} (H_{nn'} - EO_{nn'})b_{n'} = 0 \qquad n = 1, 2, ..., N \tag{4}$$

where N is the number of basis functions $\varphi_n(r)$,

$$H_{nn'} = \int \varphi_n{}^{+}(\boldsymbol{r})\, \hat{H}\varphi_{n'}(\boldsymbol{r})\, \mathrm{d}\boldsymbol{r} \tag{5}$$

$$O_{nn'} = \int \varphi_n{}^{+}(\boldsymbol{r})\,\varphi_{n'}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} \tag{6}$$

$\hat{H}$ is the system Hamiltonian and $b_{n'}$ are variational parameters.

The functions E are determined by the zeros of the secular determinant

$$\det|H_{nn'} - E\,O_{nn'}| = 0. \tag{7}$$

The principal distinction between various computational techniques reduces eventually to the choice of basis functions $\varphi_n(r)$.

In this paper, for functions $\varphi_n(r)$ we shall use the four-component spinors $\psi_n(\boldsymbol{q}, \boldsymbol{r})$ which are solutions of the Dirac equation

$$\hat{H}_0\psi_n(\boldsymbol{q}, \boldsymbol{r}) = E_n^0\psi_n(\boldsymbol{q}, \boldsymbol{r}) \tag{8}$$

Here $\boldsymbol{r}$ varies within the boundaries of a magnetic (extended) cell, and $\boldsymbol{q}$ is a wavevector from the corresponding Brillouin zone.

As the potential $V(r)$ in (2) is identical for all atoms in the extended cell, the problem of finding the energy eigenfunctions and eigenvalues in (8) may be reduced to their calculation for a one-atom cell. Let $\bar{\psi}(\boldsymbol{k}, \bar{\boldsymbol{r}})$ and $\varepsilon(\boldsymbol{k})$ denote the eigenfunctions and the corresponding energies calculated for such a one-atom cell, respectively. Since, in the absence of spin order, chromium has a BCC structure, the vectors $\boldsymbol{r}'$ and $\boldsymbol{k}$ belong to the Wigner–Seitz cell and the Brillouin zone of a BCC lattice, respectively. The electron spectrum of the extended magnetic cell is then defined as a union of spectra, $\varepsilon(\boldsymbol{k_p})$:

$$E^0(\boldsymbol{q}) = \{\varepsilon(\boldsymbol{k}_0), \varepsilon(\boldsymbol{k}_1), \ldots, \varepsilon(\boldsymbol{k}_N - 1)\}. \tag{9}$$

Here

$$\boldsymbol{k}_p = \boldsymbol{q} + \chi_p$$

and χ_p coincides in direction with the vector $\boldsymbol{Q}$, and its magnitude is defined as

$$|\chi_p| = \frac{4\pi}{a}\frac{p}{N} \qquad \text{for } p = 0, 1, 2, \ldots, N - 1$$

where N is the number of atoms in the magnetic cell.

The four-component functions $\psi(\boldsymbol{q}, \boldsymbol{r})$ can be obtained from $\bar{\psi}(\boldsymbol{k}_p, r')$ by merely using the Bloch conditions

$$\psi(\boldsymbol{q}, \boldsymbol{r}' + \boldsymbol{R}_j) = \exp(\mathrm{i}\boldsymbol{k}_p \cdot \boldsymbol{R}_j)\psi(\boldsymbol{k}_p, \boldsymbol{r}'). \tag{10}$$

The basis functions constructed in this manner automatically satisfy the necessary boundary conditions for a magnetic cell. They are orthonormal by virtue of being eigenfunctions of the Hermitian operator $\hat{H}_0$, therefore the overlapping integrals (6) take the form

$$\int \psi_n{}^{+}(\boldsymbol{q}, \boldsymbol{r})\psi_{n'}(\boldsymbol{q}, \boldsymbol{r})\,\mathrm{d}\boldsymbol{r} = \delta_{nn'}. \tag{11}$$

The solutions $\Psi(\boldsymbol{q}, \boldsymbol{r})$ of the Dirac equation (1) for the SDW are represented as a linear combination of $\psi_n(\boldsymbol{q}, \boldsymbol{r})$ with variational parameters b_n:

$$\Psi(\boldsymbol{q}, \boldsymbol{r}) = \sum_n b_n\psi_n(\boldsymbol{q}, \boldsymbol{r}) \tag{12}$$

Since it is the d electrons that are responsible for the formation of AF order in Cr, it would be reasonable to take into account in equation (12) only the energy bands with addition of 3d electrons. In view of double degeneracy, the number of such bands is $12N$. This magnitude will determine the minimum number of basis functions to be allowed for in expansion (12).

2.1. *Calculation of matrix elements* $H_{nn'}$

Our calculations are based on the relativistic version of the KKR method [12] and, as usual, the potential is believed to have a *muffin-tin* (MT) form. Then, by virtue of the fact that, outside the MT sphere, $V(r)$ and $\Delta V(r)$ are equal to zero, and $\psi(\boldsymbol{q}, \boldsymbol{r})$ are eigenfunctions of operator $\hat{H}_0$, the matrix elements (5) can be written as

$$H_{nn'}(\boldsymbol{q}) = E^0_n(\boldsymbol{q})\delta_{nn'} + \tilde{H}_{nn'}(\boldsymbol{q}). \tag{13}$$

Here

$$\tilde{H}_{nn'}(\boldsymbol{q}) = \sum_j \int_{\Omega_{MT}} \psi^{j+}_n(\boldsymbol{q}, \boldsymbol{r}) \left(\Delta V_j(r)\, \hat{\Sigma}_z\right) \psi^j_{n'}(\boldsymbol{q}, \boldsymbol{r})\, \mathrm{d}\boldsymbol{r}. \tag{14}$$

In the relativistic KKR method the trial function inside the jth MT sphere is chosen as a linear combination of solutions of the Dirac equation in the centre-symmetrical field with variational coefficients $C^{jn}_{\kappa\mu}(\boldsymbol{q})$:

$$\psi^{(j)}_n(\boldsymbol{q}, \boldsymbol{r}) = \sum_{\kappa\mu} \mathrm{i}^l C^{jn}_{\kappa\mu}(\boldsymbol{k}) \begin{pmatrix} g^{jn}_\kappa(r)\varphi_{\kappa\mu}(\hat{r}) \\ -\mathrm{i} f^{jn}_\kappa(r)\varphi_{\bar{\kappa}\mu}(\hat{r}) \end{pmatrix}. \tag{15}$$

Here κ is a quantum number such that $\kappa = l$ if $\kappa > 0$, and $\kappa = -(l+1)$ if $\kappa < 0$; $\bar{\kappa} = -\kappa$ and $\varphi_{\kappa\mu}$ are spherical spinors. $g^{jn}_\kappa(r)$ and $f^{jn}_\kappa(r)$ are the solutions of the set of radial equations

$$\begin{aligned} (g^{jn}_\kappa(r))' &= \left(1 + \frac{E - V^{(j)}(r)}{c^2}\right) c f^{jn}_\kappa(r) - \frac{\kappa+1}{r} g^{jn}_\kappa(r) \\ (c f^{jn}_\kappa(r))' &= \frac{\kappa-1}{r} c f^{jn}_\kappa(r) - [E - V^{(j)}(r)] g^{jn}_\kappa(r) \end{aligned} \tag{16}$$

and c is the velocity of light.

As the potential $V(r)$ is identical for all the atoms in the magnetic cell, the functions $g_\kappa(r)$ and $f_\kappa(r)$ do not depend on the atom number and may be calculated only once for each k. In what follows the index j on the functions $g^n_\kappa(r)$ and $f^n_\kappa(r)$ will be dropped.

Substituting (15) into (14) yields the following explicit expression for $\tilde{H}_{nn'}(\boldsymbol{q})$:

$$\begin{aligned} \tilde{H}_{nn'}(\boldsymbol{q}) = \sum_j \sum_{\kappa\mu} C^{jn^*}_{\kappa\mu}(\boldsymbol{q}) C^{jn'}_{\kappa\mu}(\boldsymbol{q}) &\left[\frac{2\mu}{2\kappa-1} \int_0^{r_{S_j}} r^2 f^n_\kappa(r)\, \Delta V_j(r)\, f^{n'}_\kappa(r)\, \mathrm{d}r \right. \\ &\left. - \frac{2\mu}{2\kappa+1} \int_0^{r_{S_j}} r^2 g^n_\kappa(r)\, \Delta V_j(r)\, g^{n'}_\kappa(r)\, \mathrm{d}r \right] \\ &- C^{jn*}_{\bar{\kappa}+1,\mu}(\boldsymbol{q}) C^{jn'}_{\kappa\mu}(\boldsymbol{q}) \left[\beta^- \int_0^{r_{S_j}} r^2 f^n_{\bar{\kappa}+1}(r) \Delta V_j(r)\, f^{n'}_\kappa(r)\, \mathrm{d}r \right] \\ &+ C^{jn^*}_{\bar{\kappa}-1,\mu}(\boldsymbol{q}) C^{jn'}_{\kappa\mu}(\boldsymbol{q}) \left[\beta^+ \int_0^{r_{S_j}} r^2 g^n_{\bar{\kappa}-1}(r) \Delta V_j(r)\, g^{n'}_\kappa(r)\, \mathrm{d}r \right] \end{aligned} \tag{17}$$

Here

$$\beta^\pm = 2\sqrt{\frac{\kappa + \mu \pm \frac{1}{2}}{2\kappa \pm 1}} \sqrt{\frac{\kappa - \mu \pm \frac{1}{2}}{2\kappa \pm 1}}$$

and r_{S_j} is the radius of the jth MT sphere.

Thus the matrix elements $\tilde{H}_{nn'}(\boldsymbol{q})$ include four terms, the first two terms involving the solutions of the set of radial equations (16) with the same value of κ. The last term relates the states with different values of κ and $-\kappa - 1$, and the same value of the orbital number l. As to the third term, it mixes the states κ and $-\kappa + 1$ corresponding to l and $l \pm 2$, respectively. Note that also in the standard spin-polarized KKR method the set of radial equations involves a term relating l and $l \pm 2$ which is neglected [11, 13]. Unlike those papers, we need not do this.

Since in the relativistic KKR method the wavefunctions are defined only inside the MT sphere, difficulties emerge in calculating integrals (11). In this work, when normalizing the wavefunctions, the following relations have been used to define the normalized KKR coefficients $C^{jn}_{\kappa\mu}(\boldsymbol{q})$ [14]:

$$\sum_{j,\kappa\mu} |C^{jn}_{\kappa\mu}|^2 = -\frac{1}{\partial\lambda_i/\partial E} \sum_{\kappa\mu} \frac{\left(\int_0^{r_S} (g_\kappa^2 + f_\kappa^2) r^2\,\mathrm{d}r\right) |t_{i,\kappa\mu}|^2}{\left\{\int_0^{r_S} V(r) \left[g_\kappa j_l + f_\kappa \frac{\sqrt{E_n^0}}{c} \left(j_l' + \frac{\kappa+1}{r\sqrt{E_n^0}} j_l \right) \right] r^2\,\mathrm{d}r \right\}^2}. \tag{18}$$

Here λ_i and $t_{i,\kappa\mu}$ are the ith eigenvalue and the corresponding eigenvectors of the standard KKR dispersive matrix, r_S is the radius of the MT sphere, and j_l and j_l' are Bessel functions and their derivatives $\mathrm{d}j_l(x)/\mathrm{d}x$, respectively. In deriving relation (18) in [14], the radial functions g_κ, f_κ and the functions ψ_n were assumed to be normalized to unity in the MT sphere and the unit cell, respectively.

Up to this point we have not used the explicit form of the spin-polarizing exchange potential $\Delta V_j(\boldsymbol{r})$. From here on, $\Delta V_j(\boldsymbol{r})$ will be assumed to vary in the magnetic cell as

$$\Delta V_j(\boldsymbol{r}) = \Delta\upsilon(\boldsymbol{r}) \cos(\boldsymbol{Q} \cdot \boldsymbol{R}_j) \tag{19}$$

$\Delta\upsilon(\boldsymbol{r})$ being site independent.

3. Computational results

In order to verify whether our technique works well, we have calculated the electronic structure of AF Cr for $\boldsymbol{Q} = (2/\pi)(0, 1, 0)$. As mentioned above, in this case the unit cell contains two atoms with coordinates $\boldsymbol{R}_0 = (a/2)(0, 0, 0)$ and $\boldsymbol{R}_1 = (a/2)(1, 1, 1)$, and the magnetic moments equal in magnitude but opposite in direction. As a consequence, at different lattice sites, the spin-polarizing part of potential (19) differs only in sign.

The accuracy of the technique was tested by comparing the energy eigenvalues with those obtained within the spin-polarized relativistic KKR (SPRKKR) method. We used this method in [6] to calculate the electronic structure of AF Cr. In the present calculation the potentials $V(r)$ and $\Delta V(r)$ are identical with those of [6].

The wavefunctions of equation (2) corresponding to the first 12 energy levels of the valence band were used as basis functions (12). As each energy level of non-magnetic Cr is doubly degenerate, the total number of terms in expansion (12) is 24.

The results of calculations for the points Γ $((2\pi/a)(0, 0, 0))$ and X $((2\pi/a)(0, 0.5, 0))$ of the Brillouin zone are listed in table 1. It can be seen that the energy eigenvalues differ, on the average, by 5×10^{-4} Ryd between the two calculations. Such an accuracy is quite sufficient for most applications. The qualitative picture of the electron spectrum is in complete agreement with our previous SPRKKR calculation. In particular, taking into consideration the relativistic effects results in additional lowering of symmetry and consequently in anisotropy of the electron spectrum for the [010] and [001] directions of the Brillouin zone. Although the difference between the energies of these directions is small

(∼0.05 mRyd), our calculation of the density of states and optical conductivity for Cr [6] has shown the contribution of the relativistic effects to the integral characteristics to be noticeable, in spite of their smallness.

Table 1. Electron spectrum of AF Cr at points Γ and X for $\boldsymbol{Q} = (2\pi/a)(0, 1, 0)$ (as compared with the SPRKKR method).

	E_n (Ryd)			
	Point Γ		Point X	
Band n	Present calculation	SPRKKR [6]	Present calculation	SPRKKR [6]
1	0.0924	0.0924	0.3912	0.3911
2	0.4062	0.4061	0.3968	0.3968
3	0.4063	0.4061	0.5587	0.5582
4	0.6429	0.6427	0.6173	0.6172
5	0.6431	0.6429	0.6565	0.6558
6	0.6469	0.6467	0.6567	0.6558
7	0.7860	0.7853	0.7193	0.7192
8	0.7860	0.7853	0.7196	0.7194
9	0.8871	0.8869	0.8025	0.8025
10	0.8872	0.8870	0.8395	0.8395
11	0.8921	0.8919	0.9005	0.9006

To emphasize the fundamental importance of such anisotropy we have performed a model calculation of the electron structure of AF Cr for two types of unit cell extended along the axes Y and Z, which corresponded to the longitudinal ($\boldsymbol{Q} = 2\pi/a(0, 0, 1 - \delta)$) spin-density wave ($\mathrm{SDW}_{\parallel}$) and transverse ($\boldsymbol{Q} = (2\pi/a)(0, 1 - \delta, 0)$) spin-density wave $\mathrm{SDW}_{\perp}$), respectively. Recall that the magnetic moment of the system was Z directed. Additionally, we have varied the number of atoms per unit cell: $N = 2, 4, 8, 20$ and 40, which corresponded to $\delta = 0, 0.5, 0.25, 0.1$ and 0.05, respectively. In all instances the same values of $V(r)$ and $\Delta\upsilon(r)$ were used. The spin-polarizing exchange part of the potential $\Delta V(r)$ for different atoms of the unit cell was defined according to (19). The number of terms in expansion (12) is $12N$.

Since the calculation was not self-consistent and a model potential was used, we have calculated only the band contribution to the total energy

$$E_B = \int^{E_F} E N(E)\,\mathrm{d}E. \tag{20}$$

When calculating the density $N(E)$ of states, integration over the Brillouin zone was performed by the tetrahedron method.

Figure 1 plots the difference $\Delta E_B = E_{B\perp} - E_{B\parallel}$ in band energy between $\mathrm{SDW}_{\perp}$ and $\mathrm{SDW}_{\parallel}$ as a function of the number of atoms in the unit cell. As can be seen, in all variants the magnitude of E_B is smaller for the $\mathrm{SDW}_{\parallel}$.

Although in the relativistic calculation the difference between the band energies of different SDW polarizations is insignificant, being actually at the limit of accuracy of our calculation, we can state with a fair degree of assurance that taking into account the relativistic effects in AF Cr results in the fact that the $\mathrm{SDW}_{\parallel}$ and $\mathrm{SDW}_{\perp}$ become energetically non-equivalent.

In the non-relativistic limit (at $c = 10^{20}$) the band contribution to the total energy does not depend on the SDW polarization. This is apparent from table 2 in which the numerical

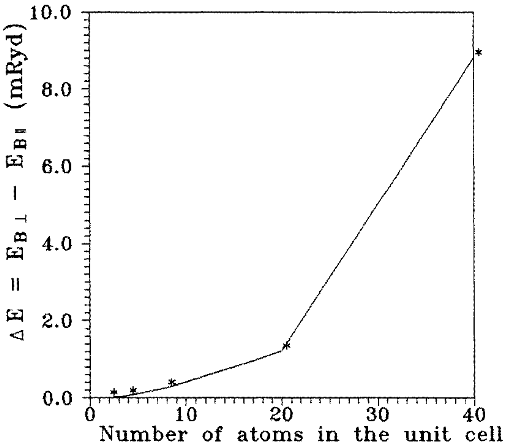

Figure 1. The difference $\Delta E_B = E_{B\perp} - E_{B\parallel}$ in band energy (per atom) between the SDW$_\perp$ and the SDW$_\parallel$ as a function of the number of atoms in the unit cell.

values of E_B for a four-atom unit cell are listed. The table also gives the values of the Fermi energy E_F and the density $N(E_F)$ of states at the Fermi level.

Table 2. Values of Fermi energy E_F, density N_{E_F} of states and band contribution E_B to the total energy for the SDW$_\parallel$ and the SDW$_\perp$ at $\delta = 0.5$ (four-atom cell). The magnetic moment is Oz-directed.

	Relativistic calculation		Non-relativistic calculation	
	SDW$_\perp$	SDW$_\parallel$	SDW$_\perp$	SDW$_\parallel$
E_F (Ryd)	0.71032	0.71030	0.71656	0.71656
$N(E_F)$ (per cell)	9.41893	9.36621	10.5092	10.5092
E_B (Ryd)	12.7067	12.7064	12.8857	12.8857

In our opinion the spin-flip (SF) phase transition occurring in AF Cr may be connected with the electron spectrum anisotropy. This transition, observed in AF Cr at 118 K, manifests itself in the fact that the longitudinal polarization of the SDW changes to the transverse polarization. From the standpoint of electronic structure, the nature of this SF transition in chromium is still unclear. Moreover, this transition is unlikely to be explained within the framework of non-relativistic treatment, the nonrelativistic electron spectra being identical for the SDW$_\parallel$ and SDW$_\perp$.

Obviously, to discuss the possibility of such a phase transition one should at least carry out a fully self-consistent calculation for different lattice constants.

4. Conclusion

Although in this paper we have used the relativistic KKR wavefunctions as basis functions, the present approach may be easily realized within any existing method for calculating the electron states. This will allow the electronic properties of materials with a complex magnetic structure to be readily calculated without loss of accuracy. The present technique, being most efficient for SDW-type systems, can also be used for helical magnetic structures. In the latter case, however, the spin-polarizing part of potential (19) should be appropriately redefined. The calculation of various matrix elements of the type

$$A_{ij} = \int \Psi^{+} \hat{A} \Psi \, \mathrm{d}r \tag{21}$$

is also simplified since these elements are expressed in terms of the sum of matrix elements calculated for trial functions, which generally is much simpler.

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