Temperature-dependent bandstructure of bulk EuO

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Abstract

We present calculations for the temperature-dependent electronic structure of bulk ferromagnetic EuO based on a parametrization of the $d-f$ model Hamiltonian using results of first-principles TB-LMTO band structure calculations. The presented method avoids the problem of double-counting of relevant interactions and takes into account the symmetry of the atomic orbitals. It enables us to determine the temperature-dependent band structure of EuO over the entire temperature range.

Key words: A. magnetically ordered materials, A. semiconductors, D. electronic band structure

The model of choice for describing the electronic and magnetic properties of magnetic rare-earth systems is the $s$-$f$ (or $s$-$d$) model [1]. The model describes the exchange coupling of itinerant band electrons to localized magnetic moments. It is applicable to the magnetic semiconductors as the europium chalcogenides and to the metallic elemental rare earths Gd, Tb, and Dy. Many characteristics of these materials can be explained by a correlation between the localized magnetic $4f$-states and extended conduction band states, mainly $5d$-$6s$. Within the $s$-$f$ model, the correlation is represented by an intraatomic exchange interaction.

There have been earlier works on the temperature-dependent band structure of bulk EuO [2,3]. The presented approach employs a decomposition of the relevant Eu-$5d$ bands of EuO into five consecutive bands. For each of these bands, a single-band $s$-$f$ model calculation has been performed. By employing this splitting procedure, the method employed by the authors [2,3] disregards the full multi-band structure of the conduction bands in EuO and leads to an overestimation of relevant correlation effects.

In the following, we will introduce a multi-band $d$-$f$ model and use it to calculate the temperature-dependent bandstructure of EuO. The employed method
combines a reliable many-body treatment of the $d$-$f$ exchange model with a self-consistent band-structure calculation. In particular, the full multi-band aspect of the problem is treated in a reliable and symmetry-conserving mode.

1 Theory

The conventional or single-band $s$-$f$ model describes the intratomic exchange interaction between an $s$-like conduction band and system of localized magnetic moments, which are due to the partially filled $4f$-shells. For a real material, like EuO, the conduction band usually consists of multiple subbands, which can be distinguished by their magnetic quantum number. In the following we will introduce the model for such a local-moment system with multiple conduction bands. The respective model will be referred to as the (multi-band) $d$-$f$ model as opposed to the (single-band) $s$-$f$ model.

The $d$-$f$ model Hamiltonian consists of three parts:

$$H = H_d + H_f + H_{df}. \tag{1}$$

For a real system like EuO, the kinetic energy of the conduction electrons reads:

$$H_d = \sum_{ijmm'} T_{ij}^{mm'} c_{ima}^+ c_{jm'\sigma}. \tag{2}$$

Here, $c_{ima}^+$ and $c_{ima}$ are, respectively, the creation and annihilation operators of an electron from the $m$-th subband at the lattice site $R_i$. $T_{ij}^{mm'}$ are the hopping integrals.

Each lattice site $R_i$ is occupied by a localized magnetic moment, represented by a spin operator $S_i$. These localized moments are exchange coupled expressed by the Heisenberg Hamiltonian:

$$H_f = \sum_{ij} J_{ij} S_i \cdot S_j, \tag{3}$$

where $J_{ij}$ are the Heisenberg exchange integrals.

In addition to the contribution of the itinerant-electron system and the contribution of the localized $f$-moments we have a third contribution to account for an intraatomic interaction between the conduction electrons and the localized $f$-spins. The form of that contribution can be derived from the general form
of the Coulomb interaction between electrons at a single lattice sites. If the
electron scattering processes caused by the Coulomb interaction are restricted
to two involved subbands $L$ and $L'$, one gets for the Coulomb interaction:

$$H_I = \frac{1}{2} \sum_{LL'\sigma\sigma'} \left[ U_{LL'} c_{L\sigma}^\dagger c_{L'\sigma'}^\dagger c_{L'\sigma'} c_{L\sigma} + J_{LL'} c_{L\sigma}^\dagger c_{L'\sigma'}^\dagger c_{L\sigma'} c_{L'\sigma} + J_{LL'}^* c_{L\sigma}^\dagger c_{L\sigma'}^\dagger c_{L'\sigma'} c_{L'\sigma} \right].$$

(4)

We can split the Coulomb interactions into three different parts, depending on
whether both $L$ and $L'$ are conduction bands, $H_I^{CC}$, both belong to localized
bands, $H_I^{LL}$, or there is an interaction between localized and conduction bands
involved, $H_I^{CL}$,

$$H_I = H_I^{CC} + H_I^{LL} + H_I^{CL}.$$  

(5)

The first of the three parts disappears, since for the case of a semiconductor
the conduction bands are unoccupied. The second term is already contained in
the description of the localized moments via the Heisenberg model in Eq. (3).
The third term is the only one which contains an interaction between the
localized bands and the conduction bands. Assigning the indices $m$ and $f$
itinerant and localized bands, respectively, it can be written in the form:

$$H_I^{CL} = \sum_{mf\sigma\sigma'} \left[ U_{mf} c_{m\sigma}^\dagger c_{f\sigma'}^\dagger c_{f\sigma'} c_{m\sigma} + J_{mf} c_{m\sigma}^\dagger c_{f\sigma'}^\dagger c_{m\sigma'} c_{f\sigma} + \frac{1}{2} (J_{mf}^* c_{m\sigma}^\dagger c_{m\sigma'}^\dagger c_{f\sigma'} c_{f\sigma} + J_{mf}^* c_{f\sigma}^\dagger c_{f\sigma'}^\dagger c_{m\sigma'} c_{m\sigma}) \right].$$

(6)

The last two terms of the above equation vanish for the special case of EuO,
due to the two fact that in Eu the localized $4f$ shell has its maximum spin of
$S = 7/2$ resulting in no double occupancy of the different subbands of the $4f$
shell. Introducing the Pauli spin operators $\sigma_L$ one arrives at

$$H_I^{CL} = -2 \sum_{mf} J_{mf} \sigma_m \cdot \sigma_f.$$  

(7)

By defining the spin operator of the local moment by $S = \hbar \sum f \sigma_f$ and by
assuming the inter-band exchange to be independent on the band indices $m$
and $f$, $J_{mf} \equiv J/2$, the multi-band $d$-$f$ interaction which is the sum of Eq. (7)
over all the different lattice sites reads:

$$H_{df} = -\frac{J}{\hbar} \sum_{im} \sigma_{im} \cdot S_i.$$  

(8)

where $J$ is the intraatomic $d$-$f$ exchange interaction. Using the second-quantized
form of $\sigma_i$ and the abbreviations

$$S_j^\sigma = S_j^x + i z_\sigma S_j^y, \quad z_{\uparrow(\downarrow)} = \pm 1,$$

(9)

the $d$-$f$ Hamiltonian can be written as

$$H_{df} = -\frac{J}{2} \sum_{ima} (z_\sigma S_i^z n_{ima} + S_i^\sigma c_{ima}^+ c_{ima}).$$

(10)

The most decisive part of the $d$-$f$ Hamiltonian (10) is the second term, which describes spin exchange processes between the conduction electrons (2) and the localized moments (3).

The many-body problem that arises with the Hamiltonian (1) is far from being trivial and a full solution is lacking. In previous papers we have presented an approximate treatment for single-band $s$-$f$ model in a local-moment system with film geometry for the special case of an empty conduction band, $n = 0$ [4]. For this special case, the approach for the single-band $s$-$f$ model in a film geometry with inequivalent layers $\alpha$ can be identically transferred to the situation of the multi-band $d$-$f$ model in bulk materials with different subbands $m$, via the index transition $\alpha \to m$. Using this transition, in the following we want to present the main results of the theoretical approach for the multi-band $d$-$f$ model.

Due to the empty conduction bands we are considering throughout the whole paper, the Hamiltonian (1) can be split into an electronic part, $H_d + H_{df}$, and a magnetic part, $H_f$, which can be solved separately [4]. For the magnetic subsystem $H_f$ we employ an approach based on the random phase approximation (RPA) which has been described in detail in [5]. As the result one gets the temperature-dependent magnetizations of the local-moment system.

Concerning the electronic subsystem, $H_d + H_{df}$, all physically relevant information can be derived from the retarded single-electron Green function

$$G_{ij\sigma}^{mm'}(E) = \left\langle \left\langle c_{ima}^+ c_{jm'a}^\sigma \right\rangle \right\rangle_E$$

$$= -i \int_0^\infty dt e^{-\frac{i}{\hbar}Et} \left\langle [c_{ima}(t), c_{jm'a}^+ (0)]^+ \right\rangle.$$

(11)

The Fourier transform of the single-electron Green function, $G_{k\sigma}^{mm'}(E) = N^{-1} \sum_{ij} e^{ik(R_i - R_j)} G_{ij\sigma}^{mm'}(E)$, is related to the spectral density via

$$S_{k\sigma}^{mm'}(E) = -\frac{1}{\pi} \text{Im} G_{k\sigma}^{mm'}(E),$$

(12)
from which the partial density of states of the \( m \)-th subband can be obtained:

\[
\rho^m_\sigma(E) = \frac{1}{\hbar N} \sum_k S^{mm}_k(E). \tag{13}
\]

For the solution of the many-body problem posed by the Hamiltonian \( H_d + H_{df} \) we write down the equation of motion of the single-electron Green function (11)

\[
E G^{mm'}_{ij\sigma} = \hbar \delta_{mm'} \delta_{ij} + \sum_{km''} T^{mm''}_{ik \sigma} G^{mm''}_{kj\sigma} + \langle \langle [c_{im\sigma}, H_{df}]_– ; c^+_{jm'\sigma} \rangle \rangle_E, \tag{14}
\]

The formal solution of Eq. (14) can be found by introducing the self-energy \( M^{mm'}_{ij\sigma}(E) \),

\[
\langle \langle [c_{im\sigma}, H_{df}]_– ; c^+_{jm'\sigma} \rangle \rangle_E = \sum_{km''} M^{mm''}_{ik\sigma}(E) G^{mm''}_{kj\sigma}(E), \tag{15}
\]

which contains all information about the correlations between the conduction band and localized moments. After combining Eqs. (14) and (15) and performing a Fourier transform we see that the formal solution of Eq. (14) is given by

\[
G_k^{\sigma}(E) = \hbar (E I - T_k - M_k^{\sigma}(E))^{-1}, \tag{16}
\]

where \( I \) represents the \((M \times M)\) identity matrix and where \( M \) is the number of subbands of the conduction-band system and where the matrices \( G_{k\sigma}(E) \), \( T_k \), and \( M_{k\sigma}(E) \) have as elements the subband-dependent functions \( G^{mm'}_{k\sigma}(E) \), \( T^{mm'}_{k} \), and \( M^{mm'}_{k\sigma}(E) \), respectively.

The evaluation of the higher Green functions resulting from (14) employs a moment-conserving decoupling approximation (MCDA). Following the steps presented in \([4]\) one arrives at an implicit set of equations for the local self-energy, \( M^{mm'}_{k\sigma}(E) \equiv \delta_{mm'} M^m_\sigma(E) \):

\[
M^m_\sigma(E) = -\frac{J}{2} \mu^m_\sigma(E), \quad \mu^m_\sigma(E) = \frac{Z^m_\sigma(E)}{N^m_\sigma(E)}, \tag{17}
\]

where the numerator and the denominator, respectively, are given by

\[
Z^m_\sigma = z_\sigma \hbar^2 \langle S^z \rangle + \frac{J}{2} \left\{ (\kappa^{(2)}_\sigma - \hbar^2 S(S + 1)) G^{mm} \right. \\
\left. - \left[ (\lambda^{(1)}_\sigma + \lambda^{(2)}_\sigma + z_\sigma \mu^m_\sigma) \hbar (S^z) + \hbar \kappa^{(2)}_\sigma G^{mm}_{0-\sigma} \right] \right\}
\]
\[
+ \frac{J^2}{4} \left\{ z_\sigma \hbar^2 S(S + 1)(\lambda^{(1)}_\sigma + \lambda^{(2)}_\sigma + z_\sigma \mu^{m}_{-\sigma}) \\
+ \kappa^{(2)}_\sigma (\mu^{m}_{\sigma} - \mu^{m}_{-\sigma}) \right\} G_{0\sigma}^{m m} G_{0-\sigma}^{m m},
\]

\[
N_{\sigma}^{m} = \hbar^2 - \frac{J}{2} \left\{ (\hbar + z_\sigma \lambda^{(2)}_\sigma + \mu^{m}_{\sigma}) G_{0\sigma}^{m m} + (z_\sigma \lambda^{(1)}_\sigma) \\
+ \mu^{m}_{-\sigma}) G_{0-\sigma}^{m m} \right\} + \frac{J^2}{4} \left\{ (\mu^{m}_{\sigma} + \hbar)(\mu^{m}_{-\sigma} + z_\sigma \lambda^{(1)}_\sigma) \\
+ z_\sigma \lambda^{(2)}_\sigma (\mu^{m}_{-\sigma} + \hbar) \right\} G_{0\sigma}^{m m} G_{0-\sigma}^{m m},
\]

where

\[
\kappa^{(1)}_\sigma = 0, \quad \kappa^{(2)}_\sigma = \langle S^{-\sigma} S^{\sigma} \rangle - \lambda^{(2)}_\sigma \langle S^{z} \rangle,
\]

\[
\lambda^{(1)}_\sigma = \frac{\langle S^{-\sigma} S^{\sigma} S^{z} \rangle + z_\sigma \langle S^{-\sigma} S^{\sigma} \rangle}{\langle S^{-\sigma} S^{\sigma} \rangle},
\]

\[
\lambda^{(2)}_\sigma = \frac{\langle S^{-\sigma} S^{\sigma} S^{z} \rangle - \langle S^{z} \rangle \langle S^{-\sigma} S^{\sigma} \rangle}{\langle (S^{z})^2 \rangle - \langle S^{z} \rangle^2}.
\]

contain f-spin correlation functions, which have to be calculated within the Heisenberg model.

For the limiting case of ferromagnetic saturation of the localized f-spin system \((T = 0)\), there exists an exact solution for the d-f (s-f) model with empty conduction band \((n = 0)\) [6]. In particular, the spectrum of the spin-\(\uparrow\) electron is only rigidly shifted compared to the free solution obtained for the case of vanishing s-f interaction, \(J = 0\). This means, that the spin-\(\uparrow\) spectra obtained within a ferromagnetic band-structure calculation provide the single-particle input (cf. Eq. (2)) for the d-f model calculation. Since the solution of the d-f for \(T = 0\) and \(n = 0\) is exact, the problem of double counting of relevant interactions is elegantly avoided in the presented approach.

To obtain the temperature-dependent band structure of EuO, the \(T = 0\) band structures are needed as single-particle input for the model calculations. These have been calculated for the Eu-5d bands, which in EuO dominate the conduction band, using a standard TB-LMTO program [7]. The results of these calculations will be presented in the next section.

2 Band-structure calculations

The europium chalcogenides crystallize in the fcc rock-salt structure. For EuO, the lattice constant is \(a = 5.142 \text{ Å} = 9.717 \text{ au} \) [8,9]. The electronic configurations of europium and oxygen in the state of the free atom and in the ionic
picture for EuO, respectively, are

\[
\text{free: } [\text{Eu}] = [\text{Xe}](4f)^7(6s)^2, \quad [\text{O}] = [\text{He}](2s)^2(2p)^2;
\]

\[
\text{EuO: } [\text{Eu}] = [\text{Xe}](4f)^7, \quad [\text{O}] = [\text{Ne}].
\]

In accordance with Hund’s coupling, the Eu-4f electrons couple to the maximum magnetic moment of \( S = 7/2 \). The difficulty in dealing with the 4f levels within an LDA calculation lies in their strongly localized character, which is due to a strong Coulomb interaction between the 4f electrons. As a result of the inability of the LDA to take into account the respective interactions correctly, a normal LDA calculation for EuO produces a metal with the 4f levels lying well within the conduction band.

To overcome this situation, we chose to treat the 4f moments as localized core electrons\(^1\). Fig. 1 shows the respective spin-dependent band structure of EuO. In Fig. 2, for the same calculation, the density of states is displayed. Here, the main contributions to the density of states originate from the O-2p levels, which constitute the valence band, and from the unoccupied Eu-5d levels. As a result of treating the 4f levels as core electrons, we have the correct ground state of an insulator. Clearly, the conduction-band region is dominated by the Eu-5d electrons. Thus, for the model calculations which will be performed in Sec. 3 it is a reasonable approximation to restrict the single-particle input obtained within the band-structure calculations to the Eu-5d bands.

### 3 Temperature-dependent band structures

In this section the LSDA band structure of bulk EuO shall be combined with an \(d-f\) model calculation to obtain the temperature-dependent band structure. Due to the fact that within our model calculation for \( T = 0 \) the spin-\( \uparrow \) spectrum is rigidly shifted towards lower energies by the amount of \( \frac{1}{2}JS \), the obtained \(k\)-dependent hopping matrices for the spin-\( \uparrow \) electron will serve us as the input for the kinetic Hamiltonian (2). Since the solution for \( T = 0 \) is exact, the problem of double counting of relevant interactions, which usually occurs when combining first-principles and model calculations, is elegantly avoided.

The temperature comes into play via the temperature-dependent \( f\)-spin correlation functions of Eqs. (20), which can be calculated within the Heisenberg

\(^1\) For EuO, it has been shown [10] that the band structures of the relevant conduction bands obtained within such a calculation differ only slightly from those obtained within an LDA+U calculation. For the 4f system Gd the different approaches for dealing with the localized 4f moments have been reviewed by Eriksson et al.\([11]\).
Fig. 1. Spin-dependent (spin-$\uparrow$: ---, spin-$\downarrow$: - - -) band structure of bulk EuO calculated within an LSDA calculation with the $4f$ levels treated as core electrons. The horizontal dashed line represents the Fermi energy.

model for the local-moment system [10,4,5]. For the following investigations, however, the concrete shape of the magnetization curve is of lesser interest
Fig. 2. Density of states, $\rho_\sigma(E)$, of bulk EuO calculated within an LSDA calculation with the $4f$ levels treated as core electrons. The upper graph shows the total density of states, whereas the lower two display the partial density of states of the O-2$p$ and the Eu-5$d$ bands. The dotted line represents the Fermi energy. The densities of states above the Fermi energy are multiplied by a factor of three and correspond to the left $y$-axis.

and the reduced magnetization $\langle S_z \rangle / S$ has been chosen as the temperature parameter.

To calculate the temperature-dependent band structure of EuO, the $d$-$f$ exchange interaction is needed. It has been shown by several authors[12–14], that the standard LSDA band-structure calculations are quite compatible with the simple Stoner or mean-field picture, in which the exchange splitting is only slightly energy dependent. Contrary to this statement, Fig.2 implies an
energy-dependent splitting of the spectra. However, the inclusion of such an energy-dependent splitting of the spectra is not possible within the theory presented in this paper and we have to take an averaged exchange interaction for the calculation of the temperature-dependent band structures. Averaging the splitting of the spectra for the two spin directions over the energy, one arrives at an average splitting of the spectra for the two spin directions of 0.875 eV. In the mean-field approximation of the $d$-$f$ model for $T = 0$ the spin-splitting is equivalent to $JS$. With $S = 7/2$ one gets for the $d$-$f$ exchange splitting $J = 0.25$ eV. This value will be used for the further $d$-$f$ model calculations.

Fig. 3 shows the temperature-dependent spectral density of bulk EuO obtained within an $d$-$f$ model calculation with $J = 0.25$ eV. For $T = 0$ ($\langle S_z \rangle / S = 1$), the spin-$\uparrow$ spectral density agrees, except for a constant energy shift, with that obtained by the LSDA calculation. However, still for $T = 0$ but for the spin-$\downarrow$ spectrum a broadening of the dispersion curves can be observed, most notably around the $\Gamma$-point, which indicates a finite lifetime of the respective quasiparticles due to correlation effects. In this respect already the $T = 0$ spin-$\downarrow$ solution goes beyond LSDA by taking into account correlation more realistically.

For intermediate temperatures ($\langle S_z \rangle / S = 0.5$) a broadening of the dispersion curves sets in also for the spin-$\uparrow$ spectra since the spin-$\uparrow$ electron can now exchange its spin with the deviated local-moment system. For the spin-$\downarrow$ spectral density, the correlation effects, already present at $T = 0$, increase, as can be seen by the further broadening of the curves. At the same time, the spin-$\uparrow$ and the spin-$\downarrow$ spectra are shifted towards higher and lower energies, respectively, reducing the effective splitting between the two spectra. This effect continues with increasing temperature, until finally, for $T = T_C$ ($\langle S_z \rangle / S = 0$), the spectra for both spin directions are equal. Clearly, the temperature-dependent effects displayed in Fig. 3 do not comply with the simple Stoner-picture which would imply a constant energy shift of the spectra. The reason for this more complicated behavior as a function of temperature is again that in the theory, the correlation is treated in a way which goes beyond mean-field.

The mentioned shift of the spin-$\uparrow$ spectrum towards lower energies when going from $T = T_C$ down to $T = 0$ represents the red shift of the optical absorption edge in EuO[15,16]. Fig. 4 displays the densities of states obtained for different magnetizations of the $4f$ moments. It can be seen that the red shift of the optical absorption edge is due to the $4f$-$5d_{t_{2g}}$ transition. From Fig. 4 one obtains a red shift of $r_s = 0.35$ eV. This value agrees reasonably with the experimental value for the red shift of 0.27 eV [9]. Here, the agreement can be further improved when choosing the splitting of the lower edges of the LSDA Eu-$5d$ bands in Fig. 2 to calculate the $d$-$f$ exchange interaction for the model calculation.
There have been previous calculations by Nolting et al. concerning the temperature-dependent band structure of bulk EuO [2,3]. In these works, the band structure
Fig. 4. Temperature-dependent densities of states of the Eu-5d bands of bulk EuO. For $T = 0$ ($\langle S_z \rangle / S = 1$) the spectra for the two spin directions are furthest away from each other and approach each other when increasing the temperature. For $T = T_C$ ($\langle S_z \rangle / S = 0$) the densities of states for both spin directions are the same (fat lines).

of the Eu-5d bands has been split into five s-like bands with the lowest eigenstates belonging to the lowest band etc. The splitting into s-bands produces five consecutive bands of an average bandwidth of about $W = 3\text{ eV}[2,3]$.

Contrary to these works, for the calculation of Figs. 3 and 4 the full band structure of the Eu-5d bands has been taken into account, thereby respecting the symmetry of the different Eu-5d orbitals. As a result, the Eu-5d bands of bulk EuO split into the $t_{2g}$ and the $e_g$ subbands with a bandwidth of about $10\text{ eV}$ and $6\text{ eV}$, respectively. For the model calculations, the decisive entity for the magnitude of the correlation effects is the $d$-$f$ exchange interaction.
over bandwidth, $J/W$. In this respect, in the previous works [2,3] the calculated correlation effects should be slightly overestimated, considering the more “natural” band decomposition employed in this thesis.

4 Conclusion

We presented a method for calculating the temperature-dependent band-structure of a local-moment system based on a parametrization of the (multi-band) $d$-$f$ model Hamiltonian using results of first-principles TB-LMTO band structure calculations. The method has been applied to the ferromagnetic semiconductor EuO.

The presented method enables us to calculate the temperature-dependent bandstructure of EuO over the entire temperature range. A main characteristics of the approach is the avoidance of double-counting of relevant interactions for the combination of first-principles and model-calculation.

Concerning the earlier works on the temperature-dependent band structure of bulk EuO [2,3], the method presented in this paper has two main advantages:

1. The full multi-band character of the conduction bands, including in particular the symmetry of the relevant orbitals, is taken into account.
2. Due to the broader bandwidths of the involved subbands the correlation effects should be treated in a more realistic fashion.

The extension of the method to systems with finite band occupation, $n \neq 0$, and to systems with reduced dimensionality promises to give an insight into the fascinating physics at the surface of rare-earth systems [17].

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