Temperature-dependent quasiparticle conduction band structure of the EuS monolayer

2000 J. Phys.: Condens. Matter 12 9857

(http://iopscience.iop.org/0953-8984/12/48/304)

J. Phys.: Condens. Matter **12** (2000) 9857–9868. Printed in the UK PII: S0953-8984(00)12951-0

Temperature-dependent quasiparticle conduction band structure of the EuS monolayer

S Mathi Jaya†, M C Valsakumar† and W Nolting‡

† Materials Science Division, Indira Gandhi Centre for Atomic Research, Kalpakkam 603102, India

‡ Festkörpertheorie, Institut für Physik, Humboldt Universität zu Berlin, Invaliden Strasse 110, 10115 Berlin, Germany

Received 29 March 2000, in final form 18 August 2000

Abstract. The temperature-dependent quasiparticle band structure of a ferromagnetic EuS monolayer is calculated using the s–f model which combines the one-electron band structure and a many-body model evaluation. The one-electron part required for the many-body calculation was obtained from a TB-LMTO (tight-binding linear muffin-tin orbital) band-structure calculation. A suitable supercell with five layers of empty spheres was used in the band-structure calculations to obtain the Bloch energies of the monolayer. We find striking correlation effects in the quasiparticle spectrum induced by the s–f exchange interaction and also observe significant temperature effects in the spectrum. We have further calculated the quasiparticle spectrum of the bulk EuS using the same s–f model in order to compare the results with those for the monolayer and to analyse the influences of the low dimensionality on the quasiparticle spectrum of this system. The bulk spectrum also exhibits significant correlation and temperature effects. The conduction bands of the monolayer as well as the bulk EuS show red-shift with respect to temperature and the magnitude of the red-shift is found to be larger for some bands in the bulk EuS compared to that of the monolayer.

1. Introduction

Dimension-reduced systems have been studied extensively during the last few decades, as these systems exhibit many unusual properties compared to those of their bulk counterparts [1–8]. For example, Co/Pd multilayers show perpendicular magnetic anisotropy [5]. Gd films exhibit surface-enhanced Curie temperature and enhanced magnetic order [3, 4].

The understanding of the properties of these dimension-reduced systems needs rather sophisticated theoretical formulations. The local density approach to the density functional (LDA-DFT) electronic structure calculations can provide some insight into the electronic structure of these systems. However, the electron-correlation effects are not properly taken into account in the LDA-DFT and hence they cannot provide a satisfactory account of the electronic structure of these systems. Further, the temperature effects are also not included in the DFT. A satisfactory description of the electronic structure of local moment films, which is the main concern of our present study, is provided by the s–f model. The model has already been employed to obtain the quasiparticle electronic structure of a model film with an empty conduction band [9] and its temperature dependence is also reported [10]. The quasiparticle spectrum of a two-layer film with finite conduction band occupation is presented in a recent paper [11].

The extension of the above-mentioned model studies to real material films is of great interest. Hence in this paper we consider the case of a monolayer EuS film. Even though the

0953-8984/00/489857+12$30.00

fabrication of monolayer EuS is still out of reach, theoretically it can be studied by treating the monolayer as a layer of EuS in a multilayer film without interlayer hopping. Hence this study is expected to lead to further calculations on multilayer films. Unlike the earlier model calculations reported in references [9], [10] and [11], the present calculations employ realistic band-structure results (multiple bands with non-trivial dispersion) as the one-electron part required in the many-body evaluation. The observation of the field emission of spin-polarized electrons from EuS-coated tungsten [12, 13] adds additional interest to this study. However, the study of this spin-filter effect is not considered in this paper; our interest is in the quasiparticle band structure of the conduction band of the EuS film which will be of importance even in a qualitative study of the above-mentioned effect. Bulk EuS is a ferromagnetic semiconductor having a T_c of 16.3 K. The magnetism of EuS arises from the 4f levels of the Eu^{2+} ion and it falls into the category of the localized magnetic systems. In the case of the monolayer EuS film, the T_c can be expected to vary from that of the bulk. However, the precise manner in which it varies is not known. Strictly speaking, long-range magnetic order does not appear in a two-dimensional system according to the Mermin–Wagner theorem [14] as long as the exchange is purely isotropic and short ranged. However, anisotropies (example: J_x and J_y different from J_z in the Heisenberg model) are always conceivable in two-dimensional systems to give long-range magnetic order [10].

Our aim is to obtain the quasiparticle band structure (QBS) of the EuS monolayer and to make a comparison of the same with that of the bulk so that the influences of the low dimensionality on the QBS of this system can be analysed. Our interest is in the QBS of the conduction bands alone and we evaluate it using the s–f model which combines a many-body model evaluation with an *ab initio* electronic structure calculation. Starting from the Bloch band structure obtained from the tight-binding linear muffin-tin orbital (TB-LMTO) band-structure calculations [15, 16] we use many-body techniques [9, 10, 17, 18] to obtain the temperature-dependent quasiparticle band structure (QBS) and quasiparticle density of states (QDOS) of the film and the bulk EuS. We present our results in the following sections along with a brief description of the method of calculation and conclusions of the present work.

2. The s–f model for the monolayer film

The s–f model describes the system of conduction electrons exchange coupled to the localized magnetic moments residing at the lattice sites. We shall consider a two-dimensional film characterized by a Bravais lattice vector $\boldsymbol{R}_i$. Every lattice site is occupied by a localized spin S. For simplicity we assume that there is only one conduction band in the system. The total Hamiltonian of this system consists of three parts:

$$H = H_s + H_f + H_{sf}.$$

H_s describes the conduction electrons (during the model evaluation, we treat them as s electrons without any Coulomb interaction):

$$H_s = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} = \sum_{k,\sigma} \varepsilon_k c^{\dagger}_{k\sigma} c_{k\sigma}.$$

t_{ij} are the hopping integrals and ε_k are the Bloch energies.

t_{ij} and ε_k are related via

$$t_{ij} = \frac{1}{N} \sum_k \varepsilon(k) \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)}.$$

H_f describes the interaction between the localized moments and it is taken to be the Heisenberg Hamiltonian:

$$H_f = -\sum_{ij} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j.$$

H_{sf} describes the interaction between the conduction electrons and the local magnetic moments:

$$H_{sf} = -J \sum_j \boldsymbol{S}_j \cdot \boldsymbol{\sigma}_j = -\frac{1}{2} J \sum_{j\sigma} (z_\sigma S_j^z n_{j\sigma} + S_j^\sigma c_{j-\sigma}^\dagger c_{j\sigma}).$$

σ_j is the electron spin operator, $n_{j\sigma}$ is the occupation number operator and J is the exchange coupling strength. We have used the abbreviation

$$S_j^\sigma = S_j^x + \mathrm{i} z_\sigma S_j^y$$

where $z_\uparrow = +1$ and $z_\downarrow = -1$. All the required information concerning the quasiparticle spectrum of this system described by the above-stated Hamiltonian can be obtained from the retarded single-electron Green function:

$$G_{ij\sigma} = \langle\langle c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_E = -\mathrm{i} \int_0^\infty \mathrm{d}t \; \mathrm{e}^{-(\mathrm{i}/\hbar)Et} \langle [c_{i\sigma}(t), c_{j\sigma}^\dagger(0)]_+ \rangle.$$

Evaluation of this Green function starts with the formulation of its equation of motion which is written as

$$\sum_r (E\delta_{ir} - T_{ir}) G_{rj\sigma}(E) = \hbar\delta_{ij} + \langle\langle [c_{i\sigma}, H_{sf}]_-; c_{j\sigma}^\dagger \rangle\rangle_E.$$

If we define the self-energy $M_{ij\sigma}(E)$ such that

$$\langle\langle [c_{i\sigma}, H_{sf}]_-; c_{j\sigma}^\dagger \rangle\rangle_E = \sum_r M_{ir\sigma}(E) G_{rj\sigma}(E)$$

then the equation of motion is formally solved by Fourier transformation leading to

$$[E - \varepsilon(\boldsymbol{k}) - M_{\boldsymbol{k}\sigma}(E)] G_{\boldsymbol{k}\sigma}(E) = \hbar.$$

The self-energy contains all of the influences of the s–f interaction on the quasiparticle spectrum and hence it is the central quantity of our study. The evaluation of the self-energy is a lengthy procedure. The detailed derivation of the self-energy of a test electron in an otherwise empty conduction band of a bulk solid is described in our earlier publication [17]. The extension to the case of a film is reported in references [9] and [10]. Hence we will not present the details here and the reader is referred to references [9], [10] and [17] for further details. The determination of the self-energy leads to the Green function which will give the spectral density and quasiparticle density of states. The spectral density is

$$S_{\boldsymbol{k}\sigma}(E) = -\frac{1}{\pi} \mathrm{Im}(G_{\boldsymbol{k}\sigma}(E))$$

and the quasiparticle density of states is

$$\rho_\sigma(E) = \frac{1}{N} \sum_{\boldsymbol{k}} S_{\boldsymbol{k}\sigma}(E).$$

3. Evaluation of the Bloch energy

In order to evaluate the Bloch energy $\varepsilon(\boldsymbol{k})$ of the film, we used the TB-LMTO method. The crystal structure of EuS is like that of NaCl. The (001) plane of EuS is treated as the monolayer required for our study. In order to switch off the electron hopping between the layers we constructed a supercell by joining three unit cells of EuS. Treating the Eu and S atoms present in the bottommost and topmost planes of the supercell as real atoms and treating all other atomic sites as empty spheres (ES), we calculated the band structure of this supercell. The supercell used in the calculation is shown in figure 1. It is a tetragonal cell with $a = b = a_0/\sqrt{2}$ and $c = 3a_0$, where a_0 is the lattice parameter of the bulk EuS. The five layers of empty spheres existing between the topmost and bottommost planes of the supercell eliminate the hopping between the layers containing real atoms. The Bloch energies in the Γ–Z direction of the supercell are found to be without any dispersion and hence the calculation gives us essentially the 2D band structure. Collecting all the wavevectors with k_x- and k_y-components we obtained the 2D band structure of the EuS film. The Bloch band structure of the bulk EuS was again calculated using the TB-LMTO method considering the experimental lattice parameter.

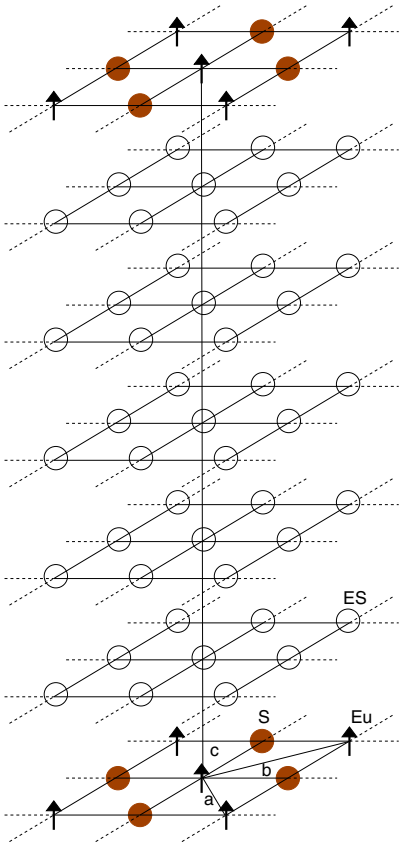

Figure 1. The supercell used to obtain the band structure of monolayer EuS.

The main problem that arises when the one-electron energies obtained from the band-structure calculations are used as the one-electron part of the many-body Hamiltonian is the possible double counting of the s–f interaction, once in an averaged way in the band-structure

calculations and then explicitly in the many-body procedure. We circumvent this problem by exploiting the fact that the spin-polarized band-structure calculations are practically consistent with the Stoner model [19, 20]. In the paramagnetic phase the Stoner quasiparticle energies are thus identical to the 'free' Bloch energies. This obviously means that the spin-induced splitting of the conduction band is absent in the paramagnetic phase. Hence we have calculated the band structure of the paramagnetic EuS monolayer and we believe that all interactions responsible for the 4f-induced magnetic behaviour of the conduction bands are then more or less switched off while all the other non-magnetic interactions are taken care of by the band-structure calculations.

The calculated band structure of the EuS monolayer is shown in figure 2. It may be seen from the figure that the conduction band has very little hybridization with the narrow 4f bands. We are interested in the quasiparticle dispersion of the conduction band alone. The conduction band is composed of six subbands. In order to treat this multiband situation we adopted the following procedure. At every $\boldsymbol{k}$-vector the energies of the six conduction bands are arranged in ascending order. The first value at every $\boldsymbol{k}$-point is taken to constitute the first conduction band and the second value at every $\boldsymbol{k}$-point to constitute the second band and so on. The six conduction bands thus obtained may be seen in figure 2 where we have shown them in different line styles. The corresponding densities of states of each of the conduction bands are shown in figure 3. The six conduction bands of the bulk EuS were also obtained in a similar way and they are shown in figure 4 along with the corresponding densities of states. Comparison of figures 2, 3 and 4 indicates that the widths of the bands are decreased in the case of the monolayer and that the density of states of the monolayer exhibits a dramatic change from that of the bulk.

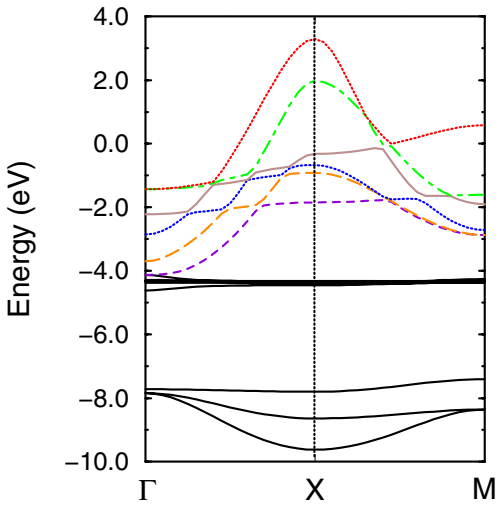

Figure 2. The conduction band structure of the EuS monolayer. The six bands are shown in different line styles.

4. Temperature dependence of the quasiparticle spectrum

Our calculations incorporate the effects of temperature on the quasiparticle spectrum. Temperature primarily enters in our calculations through the f-spin magnetization $\langle S^z \rangle$ and other spin-correlation functions such as $\langle S^- S^+ \rangle$, $\langle (S^z)^2 \rangle$, $\langle (S^z)^3 \rangle$. The self-energy actually

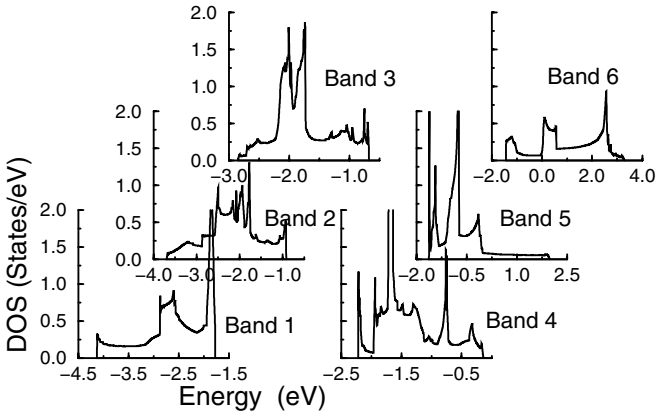

Figure 3. Densities of states of all six conduction bands of the monolayer.

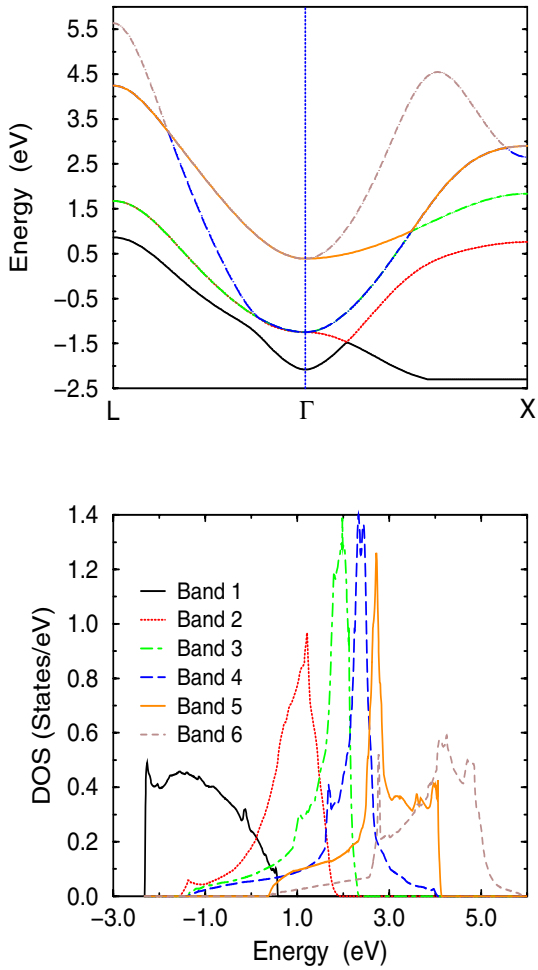

Figure 4. The conduction band structure and density of states of bulk EuS. The six bands are shown in different line styles.

involves the f-spin magnetization and all of these spin-correlation functions [10, 17, 21]. The temperature dependence of $\langle S^z \rangle$ and the spin-correlation functions thus makes the self-energy temperature dependent and hence leads to the temperature-dependent quasiparticle band structure. The conduction band of EuS is empty and hence it will have no effect on the f-spin magnetization. Thus, as regards the purely magnetic properties, EuS can be considered as a Heisenberg ferromagnet. The f-spin magnetization hence will be very close to the Brillouin function. So we assumed a Brillouin function type of behaviour for the temperature dependence of $\langle S^z \rangle$. The T_c-value of the monolayer is assumed to be the same as that of the bulk EuS as there is no experimental value of T_c available for monolayer EuS. However, this assumption will not affect our calculations except for the fact that the $\langle S^z \rangle$ at a particular temperature will correspond to another temperature if the T_c of the film is different from that of the bulk. The f-spin magnetization obtained from the Brillouin function is used to calculate the spin-correlation functions [17, 22] which are then used to calculate the temperature-dependent self-energies. These temperature-dependent self-energies are then used to obtain the temperature-dependent quasiparticle spectrum.

5. Evaluation of the self-energy and Green function

The evaluation of the self-energy is the central part of our calculations. Once the self-energy is determined, the Green function is immediately known, which will lead to the required QBS and QDOS. The self-energy in principle is a matrix with respect to the band index m which represents all six conduction subbands. However, this fact is disregarded here as the intersubband contributions are sufficiently well accounted for by the LMTO band-structure calculations. Thus we treat the six bands separately and determine the self-energies of all six bands using the procedures and formulae mentioned before and in our previous publications [17, 10, 21]. The self-energy leads to the evaluation of the Green function which gives us the spectral density and QDOS. The self-energy calculation using the bands obtained by arranging the eigenvalues in ascending order is to be considered as an approximation in our procedure. However, it is the only reliable technique for dealing with a multiband situation without much complexity. In all of our calculations the s–f exchange interaction strength is assumed to be 0.2 eV [23] and the magnitude of the f-spin moment of EuS is 7/2. The self-energies and hence the Green functions of the monolayer and the bulk EuS for all six bands were evaluated at different temperatures and the spectral density and quasiparticle density of states were subsequently evaluated. The calculated results are discussed in the following sections.

6. Discussion of results

The important results of our calculations are the QBS and QDOS and their temperature dependence. The spin-$\uparrow$ spectrum at $T = 0$ K is simple and it is identical to the 'free' Bloch dispersion shown in figure 2 except for the fact that the spectrum is shifted by a constant amount $-\frac{1}{2}JS$. Hence it is not shown here. The spin-$\downarrow$ spectrum is complicated and it exhibits in general a scattering part and a polaron part [17, 10]. The spin-down quasiparticle spectrum at $T = 0$ K is shown in figure 5 for all six conduction bands. Here we have plotted the spectral density in the form of a density plot for the wavevectors from the Γ–X and X–M directions of the 2D Brillouin zone. The intensity is a measure of the magnitude of the spectral density. The general splitting of the spectrum into two parts may be seen in the figure. The splitting is of course dependent on the coupling strength J/W, where W is the width of the Bloch band. In figure 5 the splitting is visible at some $\boldsymbol{k}$-vectors whereas there is no splitting in some

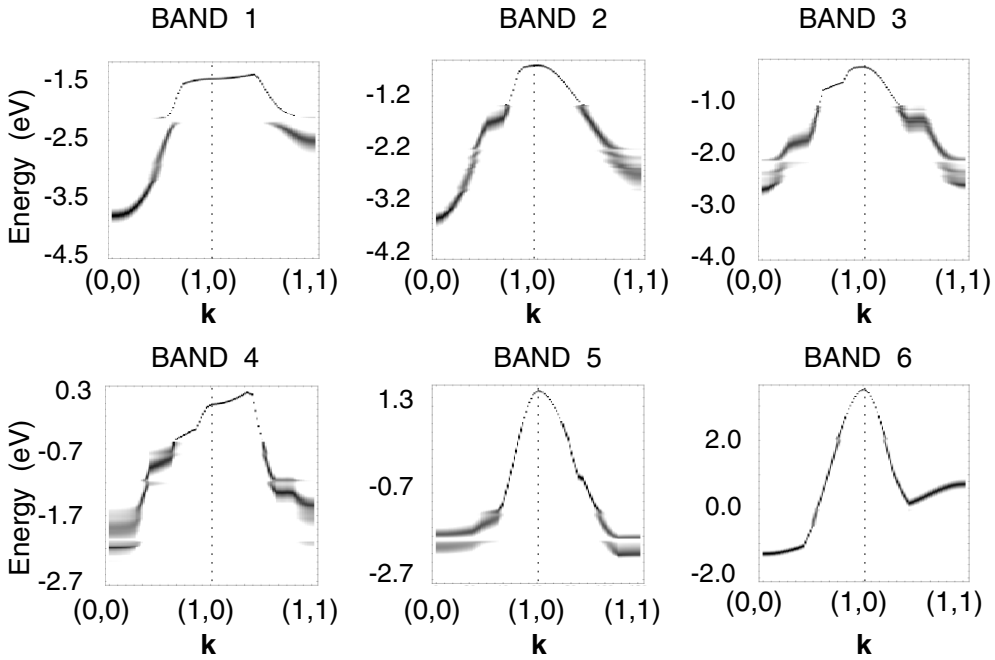

Figure 5. Spin-down quasiparticle band structure of the EuS monolayer at $T = 0$ K. ($J = 0.2$, $S = 7/2$.)

other regions of the Brillouin zone. The upper part of the split band is due to the repeated magnon emission and absorption of the conduction electrons giving rise to the formation of a magnetic polaron as discussed in our earlier papers [17, 10] and the lower part is dominated by single-magnon emission of the ↓-electron. At some $\boldsymbol{k}$-vectors the polaron part dips into the scattering part; the polaron decays into an ↑-electron plus magnon. When the J/W ratio is very small the quasiparticle dispersion looks very similar to the 'free' Bloch dispersion. In the case of the sixth conduction subband, this type of behaviour is seen.

At finite temperatures the spin-↑ spectrum also becomes complicated due to the presence of magnons in the system. The spin-↑ electron absorbs a magnon and subsequently becomes a spin-↓ electron. The magnon absorption of the spin-↑ electron is equivalent to the magnon emission by the spin-↓ electron. Hence a scattering band is formed in the spin-↑ spectrum too, as well as polaronic contributions appearing. At the same time the spectral weights are redistributed at finite temperatures and this leads to the smearing of the quasiparticle spectrum. These features may be seen in figure 6 where we have plotted the QBS for all six conduction bands at $\langle S^z \rangle / S = 0.0$. The influence of s–f correlation on the QBS may be seen by comparing figure 6 with figure 2 where we have shown the uncorrelated free Bloch dispersion of the conduction bands without any spin splitting which obviously points to the paramagnetic phase. The significant differences seen are explicitly due to the s–f correlation present in the system. Bands three and four show a splitting in the Γ–X and X–M direction plotted in the figure. Such a splitting is not at all possible in the one-electron approach.

The quasiparticle band structures of the six conduction bands of the bulk EuS were also calculated at different temperatures in order to analyse the influences of the low dimensionality on the QBS and QDOS of this system. The spin-↓ QBS at $T = 0$ K is shown in figure 7. The spin-↑ QBS is again similar to the free Bloch dispersion except for a shift of $-\frac{1}{2}JS$ and hence

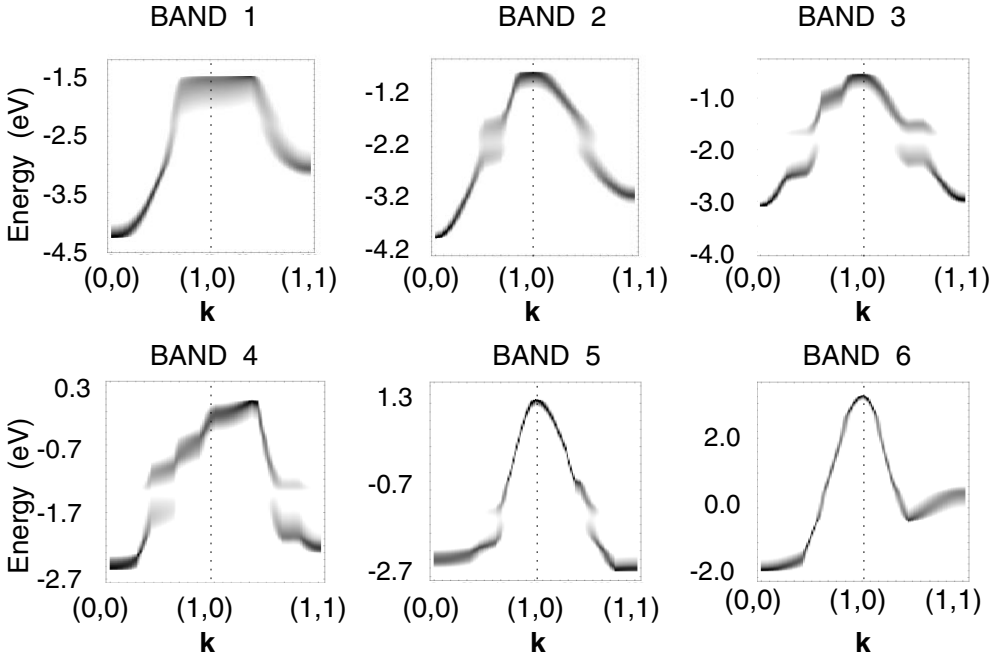

Figure 6. Quasiparticle band structure of the EuS monolayer at $T = T_c$. ($J = 0.2$, $S = 7/2$.)

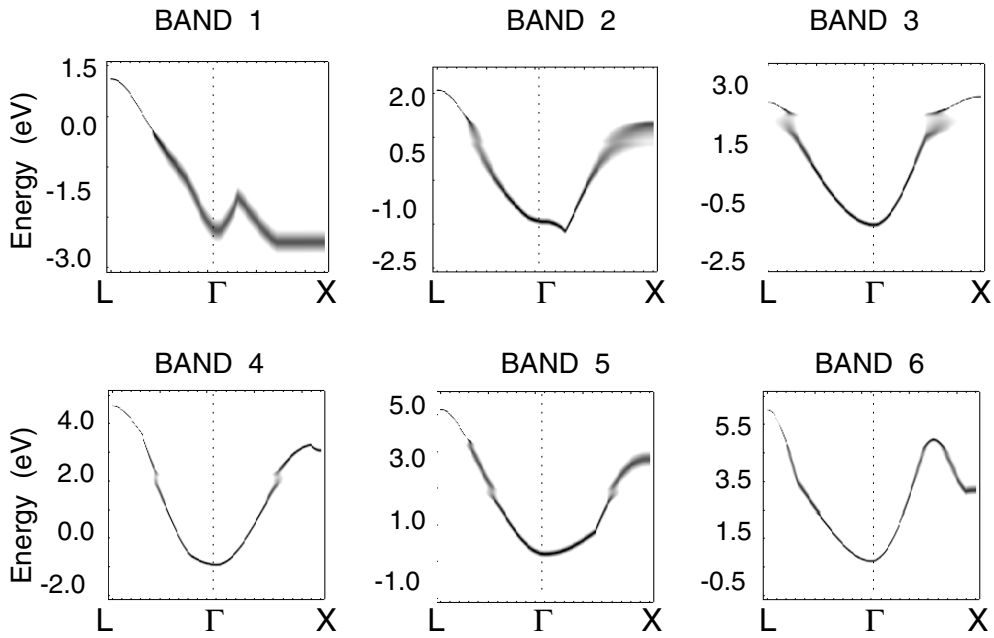

Figure 7. Spin-down quasiparticle band structure of the bulk EuS at $T = 0$ K. ($J = 0.2$, $S = 7/2$.)

it is not shown. It may be seen from the comparison of figures 4 and 7 that the QBS of the bulk EuS also exhibits significant correlation effects. Band 3 shows splitting near to the L and

X points. At finite temperatures the spectra exhibit features similar to those observed for the monolayer and hence they are not discussed.

The quasiparticle densities of states corresponding to all six conduction bands of the monolayer EuS at two different temperatures (f-spin magnetization) are shown in figure 8. The spin-up QDOS at $T = 0$ K is the same as that of the free Bloch density of states except for the shift mentioned earlier. The small deviations seen are to be attributed to the small imaginary part added to the self-energy to increase the width of the spectral density. The spin-up and spin-down spectra occupy different energy ranges at $T = 0$ K. The differences in the energy range gradually decrease with the increase of temperature and settle at the same energy range at $T = T_c$. The sharp features present in the QDOS at $T = 0$ K disappear at $T = T_c$ as the spectral weights are redistributed with the increase of temperature. The splittings of the bands three and four seen in figure 5 are not reflected in the QDOS and this obviously means that the splitting is wavevector dependent. That is, there exists splitting in some regions of the 2D Brillouin zone whereas there is no splitting in some other regions. It is known that the conduction band edge of the ferromagnetic semiconductors moves to lower values when the temperature is decreased from T_c and this effect is referred to as the red-shift. It may be seen

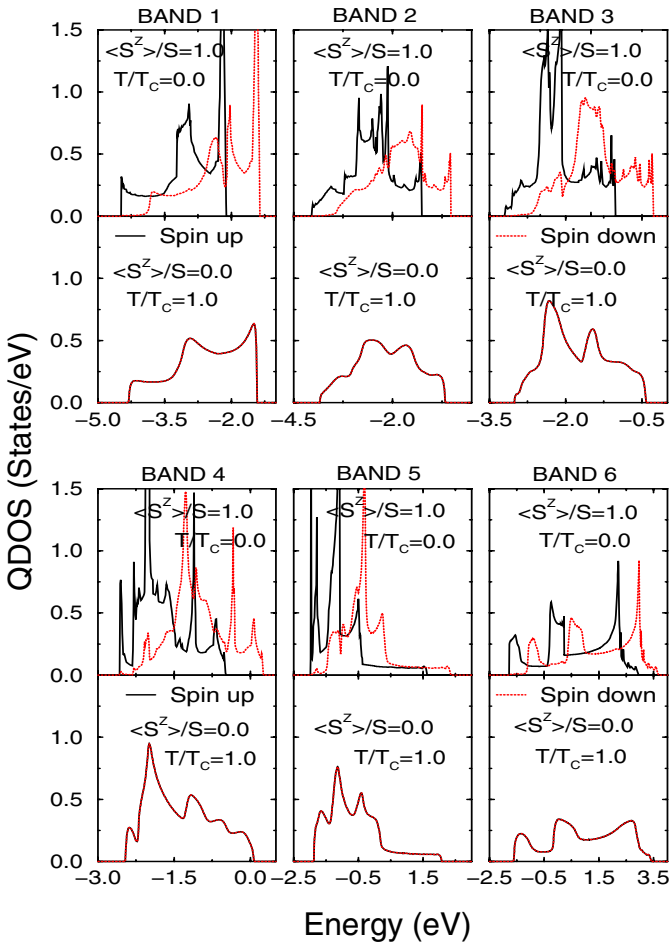

Figure 8. The quasiparticle density of states of the EuS monolayer at two different temperatures.

from figure 8 that the QDOS exhibit strong temperature dependence and all the bands exhibit red-shift with respect to temperature. The magnitude of the red-shift is found to be maximum for the third band and its value is 0.16 eV.

The QDOS of the bulk EuS is shown in figure 9. The bulk spectrum also exhibits significant correlation and temperature effects. The magnitudes of the red-shift for some bands are in fact larger compared to that of the monolayer even though the bands are broader than that of the monolayer. The densities of states of some bands of the bulk EuS are concentrated in a narrow energy range, whereas in the case of the monolayer the density of states is widely distributed and this leads to the observed behaviour of the red-shift. In the case of the first band of the bulk EuS, the density of states is widely distributed and hence it exhibits small red-shift. In any case it demonstrates its relation to the correlation strength J/W (W: effective bandwidth). The maximum red-shift is possessed by the third band and its value is 0.28 eV. The QDOS at $T = T_c$ for both the bulk and monolayer EuS is very different from the LMTO density of states which again corresponds to the paramagnetic region in the uncorrelated system. This clearly demonstrates the influence of the s–f exchange interaction on the quasiparticle spectrum.

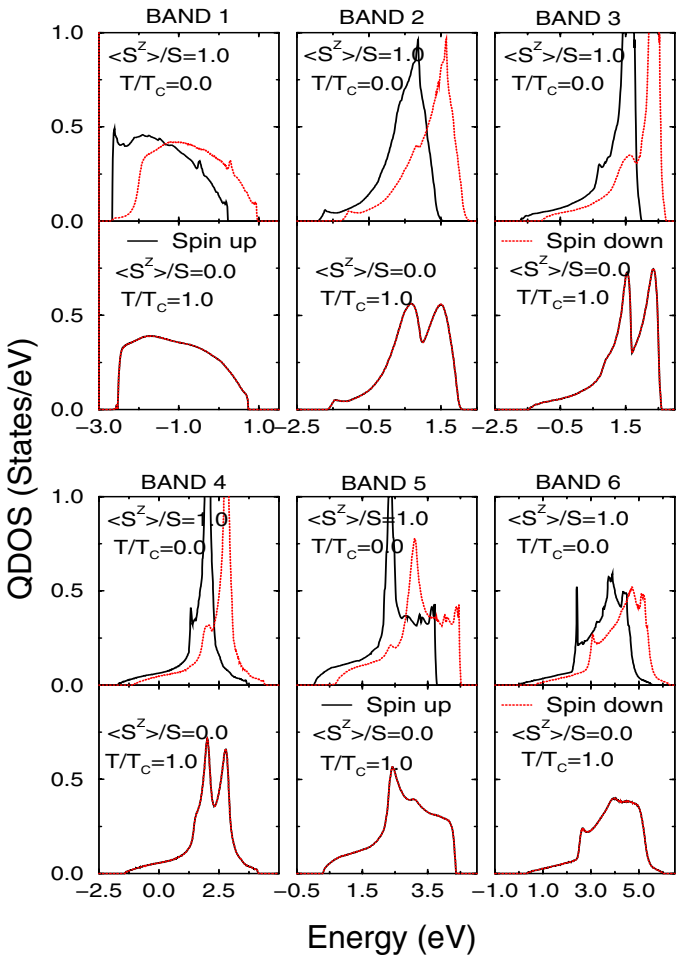

Figure 9. The quasiparticle density of states of the bulk EuS at two different temperatures.

7. Summary and conclusions

We have calculated the quasiparticle band structure of monolayer as well as bulk EuS using the s–f model. The one-electron input needed for the many-body evaluation is taken from TB-LMTO band-structure calculations. We find striking correlation effects in the quasiparticle spectrum and observe significant temperature effects also. All of the conduction bands of monolayer as well as bulk EuS exhibit red-shift with respect to decreasing temperature and the magnitude of the red-shift is found to depend on the effective coupling strength J/W. The empty conduction band as in the case of EuS film will have no effect on the f-spin system, whereas finite band occupation will have a drastic effect on the type of the magnetic order, Curie temperature and magnetization. Hence it is interesting to study the quasiparticle structure and magnetism of s–f films with finite conduction band occupation such as GdS and this will be done in a future paper.

Acknowledgment

SMJ wishes to thank IGCAR for providing him with a visiting scientist position.

References

[1] von Helmolt R, Wecker J, Holzapfel B, Shultz L and Samwer K 1993 *Phys. Rev. Lett.* **71** 2331
[2] Jin S, O'Bryan H M, Tiefel T H, McCormack M, Fastnacht R A, Ramesh R and Chen L H 1994 *Science* **264** 413
[3] Weller D, Alvarado S F, Gudat W, Shroeder K and Campagna M 1985 *Phys. Rev. Lett.* **54** 1555
[4] Tang H, Weller D, Walker T G, Scott J C, Chappert C, Hopster H, Pang A W, Dessau D S and Pappas D P 1993 *Phys. Rev. Lett.* **71** 444
[5] Weber N, Wagner K, Elmers H J, Hauschild J and Gradmann U 1997 *Phys. Rev.* B **55** 14 121
[6] Qian X and Hubner W 1999 *Phys. Rev.* B **60** 16 192
[7] Carcia P F, Meinhaldt A D and Suna A 1985 *Appl. Phys. Lett.* **47** 178
[8] Donath M, Gubanka B and Passek F 1996 *Phys. Rev. Lett.* **77** 5138
[9] Schiller R, Muller W and Nolting W 1997 *J. Magn. Magn. Mater.* **169** 39
[10] Schiller R and Nolting W 1999 *Phys. Rev.* B **60** 462
Schiller R and Nolting W 1999 *Solid State Commun.* **110** 121
[11] Mathi Jaya S and Nolting W 2000 *Physica* B **292** 359
[12] Muller N, Eckstein W, Heiland W and Zinn W 1972 *Phys. Rev. Lett.* **29** 1651
[13] Kisker E, Baum G, Mahan A H, Raith W and Reihl B 1978 *Phys. Rev.* B **18** 2256
[14] Mermin N D and Wagner H 1966 *Phys. Rev. Lett.* **17** 1133
[15] Andersen O K 1992 Methods of electronic structure calculations *ICTP Lecture Notes*
[16] Andersen O K, Pawlowska Z and Jepsen O 1986 *Phys. Rev.* B **34** 5253
[17] Nolting W, Mathi Jaya S and Rex S 1996 *Phys. Rev.* B **54** 14 455
[18] Nolting W, Mathi Jaya S and Rex S 1998 *Magnetism and Electronic Correlations in Local Moment Systems* ed M Donath, P A Dowben and W Nolting (Singapore: World Scientific)
[19] Poulsen U K, Kollar J and Andersen O K 1976 *J. Phys. F: Met. Phys.* **6** L241
[20] Janak J F and Williams A R 1976 *Phys. Rev.* B **14** 4199
[21] Mathi Jaya S and Nolting W 1997 *J. Phys.: Condens. Matter* **9** 10 439
[22] Callen H B 1963 *Phys. Rev.* **130** 890
[23] Borstel G, Borgiel W and Nolting W 1987 *Phys. Rev.* B **36** 5301