Dynamical corrections to density-functional theory for quasiparticles in ferromagnetic 4f systems. II. Finite-temperature results for EuO

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We present a theory for the temperature dependence of the electronic quasiparticle spectrum of ferromagnetic 4f systems. A concrete evaluation for the semiconductor EuO is performed and discussed. The study is based on a d-f exchange model, which has been exactly solved for $T=0$ in part I of this series. The exact solution allows us to fix the "free" Bloch energies $\varepsilon_m(\mathbf{k})$ of the model in a highly realistic manner by application of a self-consistent spin-polarized band-structure calculation based on density-functional theory. For finite temperatures the d-f model is approximately solved by a many-body procedure, which takes special care for a proper treatment of spin-exchange processes between localized 4f moments and itinerant conduction electrons. The method reproduces the exact $T=0$ limiting case. The resulting f-spin correlation functions are calculated by a moment method. We discuss in detail the one-electron spectral density for $\mathbf{k}$ vectors along the ΓL direction, real and imaginary parts of the electronic self-energy, and quasiparticle densities of states. The prominent peaks of the spectral density are used to construct a temperature-dependent quasiparticle band structure. The temperature dependence is to first order due to the magnetization, and to second order due to a transverse correlation function of the localized 4f spins.

I. INTRODUCTION

In the first paper of this series[1] (hereafter referred to as I), we presented a $T=0$ theory for the electronic quasiparticle spectrum of ferromagnetic 4f systems with special application to the semiconductor EuO. It is well known that for a qualitative understanding of such materials the so-called s-f model[2,3] has turned out to be an excellent basis. We extended this model by explicitly taking into account the 5d character of the conduction band. The decisive part of this model is an intra-atomic exchange interaction between localized 4f states and extended conduction-band states, which creates a nontrivial many-body problem. The model contains some important parameters, which have to be fixed as realistically as possible, in order to allow a direct comparison of the results to experimental data. One of these parameters is the d-f exchange matrix element. We used already in I a value ($g=0.2$ eV), which will be justified in this paper by fitting the total edge shift of the conduction band to the well-known red shift of the optical absorption edge for electronic $4f^7 5d^0 \rightarrow 4f^6 5d^1$ transitions.[4] Other very important model parameters are the one-particle Bloch energies $\varepsilon_m(\mathbf{k})$ (m = band index), which should contain in a realistic manner effects of all the other particle interactions which are not directly covered by the d-f exchange. For this purpose we performed in I a new self-consistent band-structure calculation based on the density-functional theory (DFT). The key question was, however, how to incorporate the DFT results into the d-f model without counting interactions twice. The answer was found by performing an exact $T=0$ calculation for the d-f model. In the ferromagnetic saturation the energy spectrum of spin-up quasiparticles becomes rather trivial. If we assume an empty conduction band ($n=0$), being surely realistic for EuO, then the spin-up quasiparticle density of states (↑-Q-DOS) becomes identical in shape with the "free" Bloch density of states (B-DOS), only rigidly shifted by a constant energy amount. This gave us the possibility to identify the results of the above-mentioned self-consistent band-structure calculation in the spin-up case with the Bloch energies of our model, which were therewith predetermined in a highly realistic manner. They automatically involve then all electron-electron interactions which are not explicitly treated within the framework of the d-f model. Since in the $T=0$ spin-up case the d-f exchange is rather meaningless (the rigid shift of the whole spin-up spectrum is compensated by the arbitrary choice of the energy zero), no interaction was counted twice when we solved, with the so-fixed model parameters, the d-f model for the spin-down spectrum. In spite of the fact that the spin-down spectrum is nontrivial, an exact solution is possible for $T=0$ showing interesting many-body effects which we discussed in detail in I in terms of self-energies, spectral densities, quasiparticle densities of states, and quasiparticle band structures.

In this paper we extend our theory of finite-temperature effects. For $T\neq 0$ the d-f model is no longer exactly solvable, so we propose in Sec. II a many-body approach, which, however, exactly reproduces the $T=0$ theory of I. We apply our theory again to the ferromagnetic semiconductor EuO.

values as, e.g., the magnetization $\langle S^z \rangle$ or the spin correlation $\langle S_i^{\sigma} S_i^{-\sigma} \rangle$ will enter our final results. These terms are treated separately in Sec. II C.

Previous work on the subject[3,12,13] has clearly indicated that the characteristic properties of exchange models like (6) are mainly determined by the nondiagonal part of H_{ex}, which describes spin-exchange processes between conduction electrons and localized f spins. Neglecting them from the very beginning, as is sometimes done for mathematical simplicity, is surely a very inappropriate procedure. Thinking that just the opposite is necessary, we shall handle the spin-flip terms with special care. On the other hand, the diagonal "Isinglike" part of the exchange interaction H_{ex} is believed to be sufficiently well treated by relatively simple mean-field approximations. In this spirit we shall construct our approximate solution, starting with the following decomposition of the model Hamiltonian into a "free" (H_0) and an "interacting" part (H_1):

$$H = H_0 + H_1 \ , \tag{9}$$

$$H_0 = \sum_{\substack{i,j\sigma \\ m}} T_{ij}^{(m)} c_{im\sigma}^{\dagger} c_{jm\sigma} - \tfrac{1}{2} \sum_m g_m \sum_{i,\sigma} z_{\sigma} S_i^z n_{im\sigma} \ , \tag{10}$$

$$H_1 = -\tfrac{1}{2} \sum_m g_m \sum_{i,\sigma} S_i^{\sigma} c_{im-\sigma}^{\dagger} c_{im\sigma} \ . \tag{11}$$

In the following equations of motion we need the commutators

$$[c_{im\sigma}, H_0]_- = \sum_k T_{ij}^{(m)} c_{km\sigma} - \tfrac{1}{2} g_m z_{\sigma} S_i^z c_{im\sigma} \ , \tag{12}$$

$$[c_{im\sigma}, H_1]_- = -\tfrac{1}{2} g_m S_i^{-\sigma} c_{im-\sigma} \ . \tag{13}$$

Terms arising from H_0 are treated in the mean-field approximation. This yields the following approximate equation of motion of the one-particle Green function:

$$\sum_k [(E + \tfrac{1}{2} g_m \langle S^z \rangle)\delta_{ik} - T_{ik}] G_{kj\sigma}^{(m)}(E) = \hbar \delta_{ij} + \langle\langle [c_{im\sigma}, H_1]_- ; c_{jm\sigma}^{\dagger} \rangle\rangle_E \ . \tag{14}$$

The "higher" Green function on the right-hand side defines the electronic self-energy $M_{ij\sigma}^{(m)}(E)$,

$$\langle\langle [c_{im\sigma}, H_1]_- ; c_{jm\sigma}^{\dagger} \rangle\rangle_E \equiv \sum_k M_{ik\sigma}^{(m)} G_{kj\sigma}^{(m)}(E) \ , \tag{15}$$

yielding, after Fourier transformation, the formal solution

$$G_{\mathbf{k}\sigma}^{(m)}(E) = \hbar [E - \varepsilon_m(\mathbf{k}) + \tfrac{1}{2} g_m z_{\sigma} \langle S^z \rangle - M_{\mathbf{k}\sigma}^{(m)}(E)]^{-1} \ . \tag{16}$$

The goal is a well-founded approximation for the self-energy $M_{\mathbf{k}\sigma}^{(m)}(E)$, which according to (13) and (15) is mainly determined by the "spin-flip" function

$$F_{ik,j\sigma}^{(m)}(E) = \langle\langle S_i^{-\sigma} c_{km-\sigma} ; c_{jm\sigma}^{\dagger} \rangle\rangle_E \tag{17}$$

which should be handled with care because it expresses the above-mentioned spin-exchange processes between conduction electrons and f spins. The equation of motion of this function may be written as

$$EF_{ik,j\sigma}^{(m)}(E) = \langle\langle S_i^{-\sigma} [c_{km-\sigma}, H]_- ; c_{jm\sigma}^{\dagger} \rangle\rangle_E + \langle\langle [S_i^{-\sigma}, H]_- c_{km-\sigma} ; c_{jm\sigma}^{\dagger} \rangle\rangle_E \ . \tag{18}$$

Since the conduction band of a semiconductor like EuO can be considered as practically empty, the averaging in the Green functions is performed with the electron vacuum. Therefore, the second "higher" Green function on the right-hand side of (18) vanishes identically. The other function can be divided into a "free" part (according to H_0) and an "interacting" part (according to H_1). The "free" part is simplified by a mean-field decoupling:

$$\langle\langle S_i^{-\sigma} [c_{km-\sigma}, H_0]_- ; c_{jm\sigma}^{\dagger} \rangle\rangle \rightarrow \sum_p [T_{kp}^{(m)} - \tfrac{1}{2} g_m (z_{\sigma} \langle S^z \rangle + \delta_{ik}) \delta_{kp}] F_{ip,j\sigma}^{(m)} \ . \tag{19}$$

This leads to the following intermediate result:

$$\sum_p \{[E + \tfrac{1}{2} g_m (z_{\sigma} \langle S^z \rangle + \delta_{ik})]\delta_{kp} - T_{kp}^{(m)}\} F_{ip,j\sigma}^{(m)}(E) = (1 - \delta_{ik}) H_{ki,j\sigma}^{(m)}(E) - \tfrac{1}{2} g_m \delta_{ik} R_{ij\sigma}^{(m)}(E) \ . \tag{20}$$

Here we have defined

$$H_{ki,j\sigma}^{(m)}(E) = \langle\langle [c_{km-\sigma}, H_1]_- S_i^{-\sigma} ; c_{jm\sigma}^{\dagger} \rangle\rangle_E \ , \tag{21}$$

$$R_{ij\sigma}^{(m)}(E) = \langle\langle S_i^{-\sigma} S_i^{\sigma} c_{im\sigma} ; c_{jm\sigma}^{\dagger} \rangle\rangle_E \ , \tag{22}$$

where $H_{ki,j\sigma}^{(m)}(E)$ is a one-electron Green function. The spectral decomposition of this function gives evidence that its "pole structure" must be the same as for the function $G_{ij\sigma}^{(m)}(E)$, except for the different spectral weights. The exact relation (15) therefore makes the following ansatz plausible:[14,15]

$$H_{ki,j\sigma}^{(m)}(E) \overset{(i \neq k)}{\rightarrow} \sum_p M_{kp-\sigma}^{(m)}(E) F_{ip,j\sigma}^{(m)}(E) \ , \tag{23}$$

where the self-energy $M_{kp-\sigma}^{(m)}(E)$ has to be determined self-consistently within our procedure. The other "higher" Green function $R_{ij\sigma}^{(m)}(E)$, defined in Eq. (22), is treated in the same spirit. First we construct the equation of motion of this function. Terms resulting from H_0 are again decoupled by a mean-field approximation, while the remaining "higher" function is reformulated like $H_{ki,j\sigma}^{(m)}(E)$ in (23):

$$\langle\langle S_i^{-\sigma} S_i^{\sigma} c_{im\sigma} ; [H_1, c_{jm\sigma}^{\dagger}]_- \rangle\rangle_E \rightarrow \sum_k M_{kj\sigma}^{(m)}(E) R_{ij\sigma}^{(m)}(E) \ . \tag{24}$$

This procedure finally leads to the following closed set of equations:

II. MANY-BODY APPROACH

A. The *d-f* model

We briefly repeat the most important ingredients of our model, details are already presented in I. The characteristic properties of magnetic $4f$ systems like EuO are decisively influenced by an intimate correlation between the localized Eu^{2+}-$4f$ states and extended conduction-band states, which are mainly of $5d$ type.[1,5] The seven $4f$ electron of the Eu^{2+} ion form localized magnetic moments, excellently described by the Heisenberg-Hamiltonian

$$H_f = -\sum_{i,j} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j \ . \tag{1}$$

The completely delocalized conduction electrons build the second subsystem in our model:

$$H_c = \sum_{\substack{i,j,\sigma \\ m}} T_{ij}^{(m)} c_{im\sigma}^{\dagger} c_{jm\sigma} = \sum_{\substack{\mathbf{k},\sigma \\ m}} \varepsilon_m(\mathbf{k}) c_{\mathbf{k}m\sigma}^{\dagger} c_{\mathbf{k}m\sigma} \ , \tag{2}$$

where m numbers the five $5d$ subbands, $\varepsilon_m(\mathbf{k})$ are the "free" Bloch energies, and $T_{ij}^{(m)}$ the corresponding hopping integrals. As already discussed in the Introduction the $\varepsilon_m(\mathbf{k})$ are to be considered as decisive model parameters. They should be calculated in a proper one-particle basis. According to the exact Eq. (19) in I we can identify them with the $T=0$ spin-up quasiparticle spectrum of the fully interacting system. The best one-particle basis, being available at present for EuO, is therefore given by the self-consistent spin-up spin-polarized band-structure calculation, presented in our previous paper I. Figure 1 shows the calculated one-electron density of states for the first five conduction bands, labeled by $m=1,2,\ldots,5$,

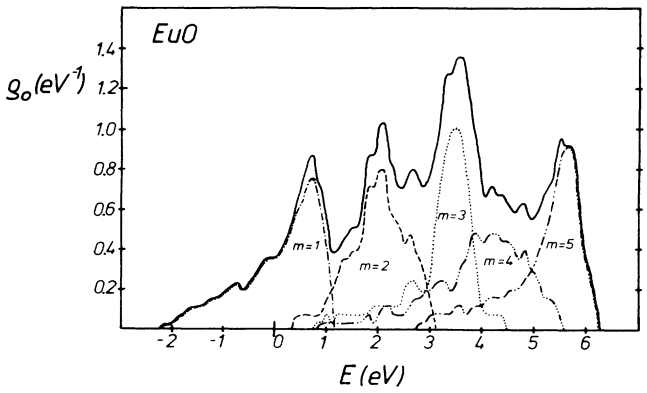

FIG. 1. Total Bloch density of states ρ_0 per atom of EuO (solid line) as a function of energy, calculated for the first five conduction bands, which are mainly of Eu^{2+}-$5d$ character. The partial densities of states ($m=1,\ldots,5$) are also indicated. The energy zero coincides with the center of gravity of the $m=1$ subband.

which are predominantly Eu^{2+}-$5d$-like. These we choose as "free" Bloch density of states (B-DOS); $\varepsilon_m(\mathbf{k})$ are then the corresponding renormalized one-particle energies. By this procedure, which only works because of the exact result (19) in I, we take automatically into account those interactions which are not explicitly contained in the *d-f* model.

The two subsystems (1) and (2) are connected by an exchange interaction of the following form:[1,3,6]

$$H_{\rm ex} = -\frac{1}{2N}\sum_{i,\sigma}\sum_{\mathbf{k},\mathbf{q}}\sum_{m,n} g_{nm}(\mathbf{k},\mathbf{k}+\mathbf{q}) e^{-i\mathbf{q}\cdot\mathbf{R}_i}\left(z_\sigma S_i^z c_{\mathbf{k}n\sigma}^{\dagger} c_{\mathbf{k}+\mathbf{q}m\sigma} + S_i^{\sigma} c_{\mathbf{k}n-\sigma}^{\dagger} c_{\mathbf{k}+\mathbf{q}m\sigma}\right) , \tag{3}$$

$$z_\sigma = \begin{cases} +1 & \text{for } \sigma=\uparrow \\ -1 & \text{for } \sigma=\downarrow \end{cases}, \quad S_j^{\sigma} = S_j^x + i z_\sigma S_j^y \ . \tag{4}$$

$g_{nm}(\mathbf{k},\mathbf{k}+\mathbf{q})$ denotes the exchange coupling, where, however, its wave-vector dependence as well as its off-diagonal elements are usually neglected,[6] excluding therewith intersubband transitions:

$$g_{nm}(\mathbf{k},\mathbf{k}+\mathbf{q}) \rightarrow g_m \delta_{nm} \ . \tag{5}$$

The total Hamiltonian of the *d-f* model

$$H = H_c + H_f + H_{\rm ex} \tag{6}$$

provokes a nontrivial many body problem, which cannot be solved exactly with the exception of some limiting cases (zero band width limit,[7] ferromagnetic saturation[1,8–11]). Our approximation is presented in Sec. II B.

B. Electronic self-energy

We want to derive reasonable expressions for basic quantities like the electronic self-energy $M_{\mathbf{k}\sigma}^{(m)}(E)$, the one-electron spectral density $A_{\mathbf{k}\sigma}^{(m)}(E)$, and the quasiparticle density of states (Q-DOS) $\rho_\sigma^{(m)}(E)$. All these terms follow directly from the (retarded or advanced) one-electron Green function

$$G_{ij\sigma}^{(m)}(E) = \langle\langle c_{im\sigma}; c_{jm\sigma}^{\dagger}\rangle\rangle_E \ , \tag{7}$$

$$G_{\mathbf{k}\sigma}^{(m)}(E) = \langle\langle c_{\mathbf{k}m\sigma}; c_{\mathbf{k}m\sigma}^{\dagger}\rangle\rangle_E = \frac{1}{N}\sum_{i,j} G_{ij\sigma}^{(m)}(E) e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)} \ . \tag{8}$$

As far as we are interested in the electronic excitation spectrum, only, we are surely allowed to neglect the magnon Hamiltonian H_f, because magnon energies are smaller by some orders of magnitude than typical electronic quantities. For this part of our theory we therefore set $H_f=0$. We shall, however, see, that as a consequence of the exchange-interaction $H_{\rm ex}$ some magnon expectation

$$\sum_k [(E+\tfrac{1}{2}g_m z_\sigma \langle S^z\rangle)\delta_{ik} - T_{ik}^{(m)}]G_{kj\sigma}^{(m)}(E) = \hbar\delta_{ij} - \tfrac{1}{2}g_m F_{ii,j\sigma}^{(m)}(E) \ , \tag{25}$$

$$\sum_p [(E-\tfrac{1}{2}g_m z_\sigma \langle S^z\rangle)\delta_{kp} - T_{kp}^{(m)} - M_{kp-\sigma}^{(m)}(E)]F_{ip,j\sigma}^{(m)}(E) + \delta_{ik}\sum_p M_{kp-\sigma}^{(m)}(E)F_{ip,j\sigma}^{(m)}(E) - \tfrac{1}{2}g_m\delta_{ik}F_{ii,j\sigma}^{(m)}(E)$$
$$= -\tfrac{1}{2}g_m \langle S_i^{-\sigma}S_i^{\sigma}\rangle \delta_{ik} G_{ij\sigma}^{(m)}(E) \ . \tag{26}$$

This can be solved by Fourier transformation. We use (8) and

$$F_{\mathbf{kp},\mathbf{q}\sigma}^{(m)} = \frac{1}{N^{3/2}}\sum_{ijk} e^{-i(\mathbf{k}\cdot\mathbf{R}_i + \mathbf{p}\cdot\mathbf{R}_k - \mathbf{q}\cdot\mathbf{R}_j)}F_{ik,j\sigma}^{(m)}(E) \ , \tag{27}$$

therewith getting a formal solution for $G_{\mathbf{k}\sigma}^{(m)}(E)$, which, compared to Eq. (16), yields the final implicit condition equation for the electronic self-energy:

$$M_\sigma^{(m)}(E) = \tfrac{1}{4}g_m^2 \langle S_i^{-\sigma}S_i^{\sigma}\rangle \frac{B_{0-\sigma}^{(m)}(E)}{1-[\tfrac{1}{2}g_m - M_{-\sigma}^{(m)}(E)]B_{0-\sigma}^{(m)}(E)} \ . \tag{28}$$

As a consequence of the neglected magnon dispersion the self-energy turns out to be wave-vector independent. $B_{0-\sigma}^{(m)}(E)$ denotes the propagator

$$B_{0\sigma}^{(m)}(E) = \frac{1}{N}\sum_{\mathbf{p}} \frac{1}{E-\varepsilon_m(\mathbf{p}) + \tfrac{1}{2}g_m z_\sigma \langle S^z\rangle - M_\sigma^{(m)}(E)} \ . \tag{29}$$

It is easy to see that our approximate theory correctly reproduces the exact $T=0$ limiting case, which we discussed extensively in our previous paper I. For, with

$$\langle S_i^{-\sigma}S_i^{\sigma}\rangle_{T=0} = \begin{cases} 0 & \text{if } \sigma = \uparrow \\ 2S & \text{if } \sigma = \downarrow \end{cases} \tag{30}$$

we find from (28)

$$M_\uparrow^{(m)}(E;T=0) = 0 \ , \tag{31}$$

$$M_\downarrow^{(m)}(E;T=0) = \tfrac{1}{2}g_m^2 S \frac{B_{0\uparrow}^{(m)}(E;T=0)}{1-\tfrac{1}{2}g_m B_{0\uparrow}^{(m)}(E;T=0)} \ , \tag{32}$$

$$B_{0\uparrow}^{(m)}(E;T=0) = \frac{1}{N}\sum_{\mathbf{p}} [E-\varepsilon_m(\mathbf{p}) + \tfrac{1}{2}g_m S]^{-1} \ . \tag{33}$$

This agrees with Eqs. (24) and (25) in I. We consider this agreement of our approximate theory with the exact solution of the nontrivial $T=0$ case as a weighty argument for our procedure.

Physical quantities of special importance for our further study are the one-electron spectral density

$$A_{\mathbf{k}\sigma}^{(m)}(E) = -\frac{1}{\pi}\mathrm{Im}G_{\mathbf{k}\sigma}^{(m)}(E+i0^+) \tag{34}$$

and the quasiparticle density of states

$$\rho_\sigma^{(m)}(E) = \frac{1}{N\hbar}\sum_{\mathbf{k}} A_{\mathbf{k}\sigma}^{(m)}(E) \ . \tag{35}$$

In general, the electronic self-energy $M_\sigma^{(m)}(E)$ will be a complex quantity

$$M_\sigma^{(m)}(E) = R_\sigma^{(m)}(E) + iI_\sigma^{(m)}(E) \ , \tag{36}$$

so that with (16) and (34) the spectral density reads as

$$A_{\mathbf{k}\sigma}^{(m)}(E) = \frac{\hbar}{\pi}\frac{0^+ - I_\sigma^{(m)}(E)}{[E-R_\sigma^{(m)}(E) + \tfrac{1}{2}g_m z_\sigma \langle S^z\rangle - \varepsilon_m(\mathbf{k})]^2 + [0^+ - I_\sigma^{(m)}(E)]^2} \ . \tag{37}$$

The wave-vector summation in (35) may be replaced by an energy integration, if one introduces the Bloch density of states (B-DOS) $\rho_0^{(m)}(E)$

$$\rho_0^{(m)}(E) = \frac{1}{N}\sum_{\mathbf{k}} \delta(E-\varepsilon_m(\mathbf{k})) \ . \tag{38}$$

For the Q-DOS we have then to evaluate

$$\rho_\sigma^{(m)}(E)=\rho_0^{(m)}(E-R_\sigma^{(m)}(E)+\tfrac{1}{2}g_m z_\sigma\langle S^z\rangle) \quad \text{if } I_\sigma^{(m)}\equiv 0 \ , \tag{39}$$

$$\rho_\sigma^{(m)}(E)=-\frac{1}{\pi}I_\sigma^{(m)}(E)\int_{-\infty}^{+\infty}dx\rho_0^{(m)}(x)\{[E-R_\sigma^{(m)}(E)+\tfrac{1}{2}g_m z_\sigma\langle S^z\rangle-x]^2+[I_\sigma^{(m)}(E)]^2\}^{-1} \quad \text{if } I_\sigma^{(m)}(E)\neq 0 \ . \tag{40}$$

According to Eq. (28) the imaginary part $I_\sigma^{(m)}$ of the self-energy is mainly determined by the imaginary part of the propagator $B_{0-\sigma}^{(m)}(E)$. Combining (16), (29), (34), and (35) we get

$$\mathrm{Im}B_{0\sigma}^{(m)}(E)=-\pi\rho_\sigma^{(m)}(E) \ . \tag{41}$$

That means that the imaginary part of the self-energy may be written as

$$I_\sigma^{(m)}(E)=\rho_{-\sigma}^{(m)}(E)F(E) \ , \tag{42}$$

where $F(E)$ is a more or less complicated function of energy E. From this relation we conclude that both spin spectra [$\rho_\sigma^{(m)}(E)$ and $\rho_{-\sigma}^{(m)}(E)$] will occupy the same energy regions, because from $\rho_{-\sigma}^{(m)}\neq 0$ follows $I_\sigma^{(m)}\neq 0$ and therewith according to (40) $\rho_\sigma^{(m)}\neq 0$ and vice versa. We shall come back to this point when discussing the results.

The above-presented general results give clear evidence how sensitively the concrete conclusions of our model will depend on a proper choice of the B-DOS, which we have derived from a self-consistent band-structure calculation based on density-functional theory as explained in Sec. II A.

The present results are, however, also very sensitively dependent on the f magnetization $\langle S^z\rangle$ as well as the intra-atomic f spin correlation $\langle S^{-\sigma}S^{\sigma}\rangle$. These quantities we determine by use of a moment method.

C. f-spin correlations

From our general results (28) and (29) it is clear, that the quasiparticle energy spectrum will exhibit a strong temperature dependence caused by the magnetization $\langle S^z\rangle$ and the transverse spin correlation $\langle S^{-\sigma}S^{\sigma}\rangle$ of the localized f system. In principle, these quantities must be derived from our model Hamiltonian (6). Since we can, however, assume for EuO an empty conduction band, it is completely sufficient to use the operator H_f, defined in Eq. (1). H_f represents the well-known, but not exactly solvable Heisenberg model. We first rewrite H_f by use of the Dyson-Maléev transformation of the spin operators[16,17]

$$S_i^- = \sqrt{2S}\,\alpha_i^\dagger \ , \tag{43}$$

$$S_i^+ = \sqrt{2S}\left[1-\frac{\alpha_i^\dagger\alpha_i}{2S}\right]\alpha_i \ , \tag{44}$$

$$S_i^z = S-\alpha_i^\dagger\alpha_i \ . \tag{45}$$

After transforming the Bose operators $\alpha_i,\alpha_i^\dagger$, as well as the exchange integrals J_{ij} to wave vectors

$$\alpha_{\mathbf{q}}=\frac{1}{\sqrt{N}}\sum_i e^{-i\mathbf{q}\cdot\mathbf{R}_i}\alpha_i \ , \tag{46}$$

$$J(\mathbf{q})=\frac{1}{N}\sum_{i,j}J_{ij}e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)} \ , \tag{47}$$

we get for the Heisenberg Hamiltonian H_f (Refs. 16 and 17)

$$H_f=-NS^2J_0+\sum_{\mathbf{q}}\hbar\omega(\mathbf{q})\alpha_{\mathbf{q}}^\dagger\alpha_{\mathbf{q}} +\frac{1}{N}\sum_{q_1,\ldots,q_4}[J(\mathbf{q}_4)-J(\mathbf{q}_1-\mathbf{q}_3)] \times\delta_{\mathbf{q}_1+\mathbf{q}_2,\mathbf{q}_3+\mathbf{q}_4}\alpha_{\mathbf{q}_1}^\dagger\alpha_{\mathbf{q}_2}^\dagger\alpha_{\mathbf{q}_3}\alpha_{\mathbf{q}_4} \ . \tag{48}$$

The second term represents noninteracting spin waves,

$$\hbar\omega(\mathbf{q})=2S[J_0-J(\mathbf{q})], \quad J_0=J(\mathbf{q}=0) \tag{49}$$

while the third term describes an interaction between them. As for the electronic system in Eq. (34) we can define for the magnon system, too, a one-particle spectral density:

$$B_{\mathbf{q}}(E)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}d(t-t')\langle[\alpha_{\mathbf{q}}(t),\alpha_{\mathbf{q}}^\dagger(t')]_-\rangle \times\exp\left[\frac{i}{\hbar}E(t-t')\right] \ . \tag{50}$$

We determine this function by a moment method,[12,13,18] which consists of two steps. First we try to find a physically reasonable ansatz for the spectral density, which should contain some free parameters. In the second step these parameters are fixed by equating the first moments $M_{\mathbf{q}}^{(n)}$ of $B_{\mathbf{q}}(E)$ via

$$M_{\mathbf{q}}^{(n)}=\frac{1}{\hbar}\int_{-\infty}^{+\infty}dE\,E^nB_{\mathbf{q}}(E) \ . \tag{51}$$

The moments are calculable, independently of the required function $B_{\mathbf{q}}(E)$, by the relation

$$M_{\mathbf{q}}^{(n)}=\langle[[\cdots[[\alpha_{\mathbf{q}},H_f]_-,H_f]_-,\ldots,H_f]_-,\alpha_{\mathbf{q}}^\dagger]_-\rangle \ . \tag{52}$$

where the square brackets enclose an n-fold commutator.

What is a reasonable ansatz for $B_{\mathbf{q}}(E)$? For very low temperature ($T\to 0$) the interaction term in (48) becomes meaningless because the system contains only very few magnons. Then

$$B_{\mathbf{q}}^{(0)}(E)=\hbar\delta(E-\hbar\omega(\mathbf{q})) \tag{53}$$

is exact. For raising temperatures, magnon interactions become non-negligible leading to a renormalization of the spin waves and to finite lifetimes of the quasiparticles. For not too high temperatures, however, magnon damping is surely not that important, so that we can assume renormalized, but real spin wave energies. A proper ansatz for the spectral density is then

$$B_{\mathbf{q}}(E)=b_{\mathbf{q}}\delta(E-\hbar\Omega(\mathbf{q})) \ , \tag{54}$$

where $b_{\mathbf{q}}$ and $\hbar\Omega(\mathbf{q})$ are at first unknown parameters,

which we fix by the first two spectral moments, using Eqs. (48), (51), and (52). This leads to

$$b_{\mathbf{q}}=\hbar \tag{55}$$

and gives an implicit condition equation for the "renormalized" spin-wave energies:

$$\hbar\Omega(\mathbf{q})=\hbar\omega(\mathbf{q})+\frac{2}{N}\sum_{\mathbf{q}_1}\frac{J(\mathbf{q})-J(0)+J(\mathbf{q}_1)-J(\mathbf{q}-\mathbf{q}_1)}{\exp[\beta\hbar\Omega(\mathbf{q}_1)]-1} . \tag{56}$$

Here we have used the spectral theorem for the expectation value $\langle\alpha^{\dagger}_{\mathbf{q}_1}\alpha_{\mathbf{q}_1}\rangle$,

$$\langle\alpha^{\dagger}_{\mathbf{q}_1}\alpha_{\mathbf{q}_1}\rangle=\frac{1}{\hbar}\int_{-\infty}^{+\infty}dE\frac{B_{\mathbf{q}_1}(E)}{\exp(\beta E)-1}$$

$$=\{\exp[\beta\hbar\Omega(\mathbf{q}_1)]-1\}^{-1} . \tag{57}$$

It is a remarkable fact that the simple ansatz (54) turns out to be completely equivalent to Dyson's famous spin-wave theory.[16,17]

If z_i is the number of f moments in the ith shell with respect to a given atom, J_i the exchange integral between ith neighbors, and

$$\gamma^{(i)}_{\mathbf{q}}=\frac{1}{z_i}\sum_{\Delta_i}e^{i\mathbf{q}\cdot\mathbf{R}_{\Delta_i}} , \tag{58}$$

where the sum runs over all magnetic sites $\mathbf{R}_{\Delta_i}$ of the ith shell, then the renormalized spin waves (56) can be cast into the form

$$\hbar\Omega(\mathbf{q})=2S\sum_i(1-\gamma^{(i)}_{\mathbf{q}})z_iJ_i[1-A_i(T)] , \tag{59}$$

$$A_i(T)=\frac{1}{NS}\sum_{\mathbf{p}}\frac{1-\gamma^{(i)}_{\mathbf{p}}}{\exp[\beta\hbar\Omega(\mathbf{p})]-1} . \tag{60}$$

It is well known[19–22] that in EuO only nearest and next-nearest neighbors interact via

$$J_1/k_B=0.625\ \text{K}, J_2/k_B=0.125\ \text{K} . \tag{61}$$

The Eu^{2+} ions occupy sites of an fcc lattice, so we have to sum in Eq. (60) over the first fcc Brillouin zone. This can be done self-consistently without further restrictions. By use of the so determined renormalized spin-wave energies $\hbar\Omega(\mathbf{q})$ we can derive the f magnetization $\langle S^z\rangle$, for which we have to evaluate according to Eqs. (45), (46) and (57) the following expression:

$$\langle S^z\rangle/S=1-\frac{1}{NS}\sum_{\mathbf{q}}\{\exp[\beta\hbar\Omega(\mathbf{q})]-1\}^{-1} . \tag{62}$$

The numerical results are excellently fitted by the expansion[23]

$$\langle S^z\rangle/S=1-0.1757t^{3/2}(1+2.9025t-1.1012t^2) , \quad t=T/T_c . \tag{63}$$

This spin-wave result is correct at least in the temperature region $0\leqq t\leqq 0.7$. In the critical region ($0.9\leqq t\leqq 1.0$) we can use a power law[20]

$$\langle S^z\rangle/S=1.17(1-t)^{0.36} . \tag{64}$$

The intermediate region ($0.7\leqq t\leqq 0.9$) is not directly accessible. We have combined the two regions (63) and (64) by the following polynomial fit:

$$\langle S^z\rangle/S=0.6571-0.1424x-0.0505x^2-0.0149x^3 , \quad x=7.6923t-6.1544 . \tag{65}$$

The full result (63), (64), and (65) for the EuO magnetization $\langle S^z\rangle/S$ is represented in the inset in Fig. 2. The agreement with the experimental data of Ref. 20 is excellent.

The determination of the transverse spin correlation function still remains:

$$\langle S_i^-S_i^+\rangle=2S(S-\langle S^z\rangle)-\frac{1}{N^2}\sum_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}\langle\alpha^{\dagger}_{\mathbf{q}_1}\alpha^{\dagger}_{\mathbf{q}_2}\alpha_{\mathbf{q}_3}\alpha_{\mathbf{q}_1+\mathbf{q}_2-\mathbf{q}_3}\rangle . \tag{66}$$

Using the spectral theorem the expectation value on the right-hand side is derivable from the following "higher" spectral density:

$$\hat{B}_{\mathbf{q}_2\mathbf{q}_3;\mathbf{q}_1}(E)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}d(t-t')\langle[\alpha^{\dagger}_{\mathbf{q}_2}(t)\alpha_{\mathbf{q}_3}(t)\alpha_{\mathbf{q}_1+\mathbf{q}_2-\mathbf{q}_3}(t),\alpha^{\dagger}_{\mathbf{q}_1}(t')]_-\rangle\exp\left[\frac{i}{\hbar}E(t-t')\right] . \tag{67}$$

Inspecting the spectral decomposition of this function one recognizes that its poles express just the energies needed for adding one additional magnon to the system. The poles are therefore the same as for the simpler function $B_{\mathbf{q}}(E)$, defined in (50), only the spectral weights are different. If we accept the one-pole ansatz for $B_{\mathbf{q}}(E)$, we have consequently to accept a one-pole ansatz for $\hat{B}_{\mathbf{q}_2,\mathbf{q}_3,\mathbf{q}_1}(E)$, too:

$$\hat{B}_{\mathbf{q}_2\mathbf{q}_3;\mathbf{q}_1}(E)=\alpha(\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3)\delta(E-\hbar\Omega(\mathbf{q}_1)) . \tag{68}$$

This ansatz contains only one additional unknown parameter, namely the spectral weight $\alpha(\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3)$, which equals just the first spectral moment of $\hat{B}$:

$$\alpha(\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3)=\hbar\langle\alpha^{\dagger}_{\mathbf{q}_2}\alpha_{\mathbf{q}_3}\rangle(\delta_{\mathbf{q}_2,\mathbf{q}_3}+\delta_{\mathbf{q}_1,\mathbf{q}_3}) . \tag{69}$$

This finally leads to the following simple result for the transverse spin correlation, surely reliable at least in the temperature region $0\leqq T/T_c\leqq 0.7$:

$$\langle S_i^{\sigma}S_i^{-\sigma}\rangle=(1+z_{\sigma})\langle S^z\rangle+(S+\langle S^z\rangle)(S-\langle S^z\rangle) . \tag{70}$$

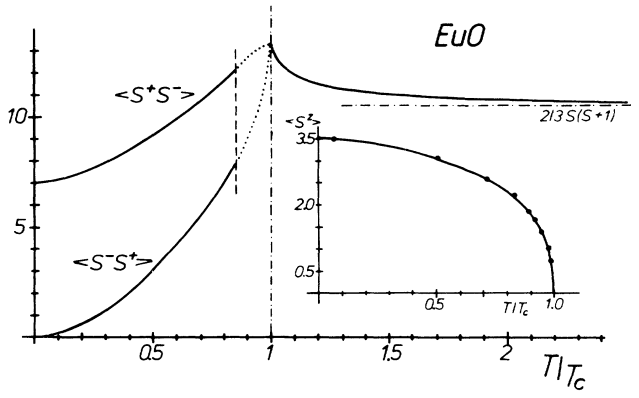

FIG. 2. Transverse intra-atomic f-spin correlation of EuO ($T_c = 69.33$ K) as a function of reduced temperature T/T_c. The low-temperature part is calculated by a moment method (Sec. II C), the high-temperature part ($T > T_c$) by the local mean-field theory of Sinkkonen (Ref. 24). The inset shows the f magnetization $\langle S^z \rangle$ as function of T/T_c. The solid line represents the theory of Sec. II C. Points are experimental data from Ref. 20.

This is plotted in Fig. 2. Unfortunately, we cannot apply the above-presented low-temperature theory in the critical and the paramagnetic region. For $T > T_c$ the formula of Sinkkonen's "local" mean-field approximation[24,25] appears sufficiently useful:

$$\langle S_i^{\sigma} S_i^{-\sigma} \rangle = \tfrac{2}{3} S(S+1) \frac{1}{N} \sum_{\mathbf{q}} \left[1 - \frac{T_c}{T} \frac{J(\mathbf{q})}{J(0)} \right]^{-1} . \tag{71}$$

The concrete evaluation of this formula for EuO is also plotted in Fig. 2.

III. DISCUSSION OF THE RESULTS

The main goal of our investigation concerns the temperature dependence of the electronic quasiparticle spectrum of the ferromagnetic semiconductor EuO. Starting point for our study is the exchange model (6), which we approximately solved by a many-body theoretical treatment. In our previous paper (I) we concentrated ourselves on the $T = 0$ solution, which could be found rigorously. We consider it as a weighty confirmation of our approximate theory that this nontrivial, exactly solvable limiting case of d-f model (6) is correctly reproduced. Our model (6) contains some important parameters. As already stressed in Sec. II A, special attention is devoted to the B-DOS $\rho_0^{(m)}(E)$. Via the exact relation (19) in I [or equivalently Eq. (21) in this paper] we were able to construct a direct connection between our many-body theory and a spin-polarized, self-consistent band-structure calculation, which permitted a really realistic determination of $\rho_0^{(m)}(E)$. The B-DOS is plotted in Fig. 1. We use this function for our further analysis. Another important model parameter is the exchange coupling constant g_m. It has been shown[3,9,26] that this quantity together with the Bloch bandwidth W_m decisively determines the temperature dependence of the quasiparticle energy spectrum. Particularly striking is the shift of the lower conduction band edge to lower energies with decreasing temperature. This effect has been observed in ferromagnetic semiconductors as red shift of the optical absorption edge for the electronic $4f^7 5d^0 \rightarrow 4f^6 5d^1$ transition.[4] The temperature dependence of the optical absorption edge of EuO, as measured by Schoenes and Wachter,[27] is plotted as a solid line in Fig. 3. This red shift effect serves to fix the exchange constant g_1. The problem, however, is that the lower edge is not uniquely defined, neither theoretically nor experimentally. We have chosen

$$g_1 = 0.2 \text{ eV} . \tag{72}$$

In spite of the fact that this value gives a slightly too high total red shift [0.28 eV instead of 0.26 eV (Ref. 27)], we believe that this is a realistic choice, because it is well known[28] that the density-functional theory gives slightly too broad bands (up to 10%). Smaller bandwidth, however, means less red shift, as is illustrated in Fig. 3. If we replace, tentatively, for an unambiguous definition of the edge shift the real $m = 1$ subband DOS (in Fig. 1) by a rectangular triangle DOS with the same area and the same height, then we get with $g_1 = 0.2$ eV a nearly exact fit of the experimental value for the total red shift. Below $0.8 T_c$ our theoretical curves for the edge shift show a realistic temperature behavior (Fig. 3) compared to the experimental data. In the paramagnetic region the calculated edge shift is always a little bit too small. This may be due to the mean-field approximation (71) for the intra-atomic transverse spin correlation.

Unfortunately we have no direct possibility to fit in a similar manner the exchange constants of th other 5d subbands. Since it is to expect that all g_m will be of the same order of magnitude, we have assumed, somewhat arbi-

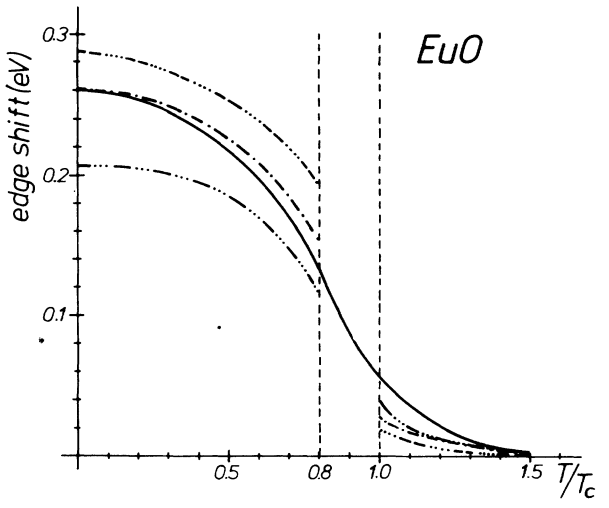

FIG. 3. Shift of the lower conduction band edge as a function of the reduced temperature T/T_c. ——: experimental data (Ref. 27); - - - - - - -: theory presented in this paper; —·—·—·: edge shift calculated with a triangle B-DOS and $W = 2$ eV; —···—···: edge shift calculated with a triangle B-DOS and $W = 1$ eV.

trarily, all g_m to be equal.

With the so fixed model parameters we have first calculated the total spin-polarized Q-DOS $\rho_\uparrow$ and $\rho_\downarrow$, which are plotted in Figs. 4 and 5 as functions of energy. We observe some drastic temperature effects, in the spin-up spectrum most remarkably in the low-energy part of the conduction band, in the spin-down spectrum more strikingly in the high-energy part. The first prominent spin-up peak, e.g., is shifted by about 1 eV to lower energies, when the crystal is cooled down from room temperature to 0 K. The second spin-up peak does not shift so much, but increases strongly with decreasing temperature. Such effects should be observable in an inverse photoemission experiment.

The temperature dependences of the two spin-polarized Q-DOS $\rho_\uparrow$ and $\rho_\downarrow$ are especially striking in the ferromagnetic phase, and then mainly caused by the f magnetization $\langle S^z \rangle$. As a consequence of the transverse spin correlation function in the expression (28) for the electronic self-energy, temperature reactions are, however, not at all restricted to the ferromagnetic phase, but happen in the paramagnetic phase, too. As already discussed in connection with Eq. (42) both spin-spectra occupy for finite temperatures exactly the same energy regions. For temperatures below the Curie point T_c, the spin-down state density is, however, very much smaller near the lower edge than the spin-up state density, so that there appears an effective exchange splitting which increases with decreasing temperature. The relative shift is not all rigid. We observe strong modifications of the original B-DOS resulting first of all from spin-exchange processes between f moments and conduction electrons mediated by the transversal part of the d-f exchange interaction (3). This part is also responsible for the temperature dependence of the Q-DOS in the paramagnetic phase.

The total Q-DOS $\rho_\uparrow$ in Fig. 4 and $\rho_\downarrow$ in Fig. 5 are simply the sums of the five corresponding partial subband densities of states $\rho_\sigma^{(m)}$, which are plotted separately in Fig. 6. The $T=0$ spin-up curves are identical in shape with the B-DOS $\rho_0^{(m)}$ because of the exact result (31). The comparison of the other curves with the original state densities $\rho_0^{(m)}$ in Fig. 1 gives evidence how strongly

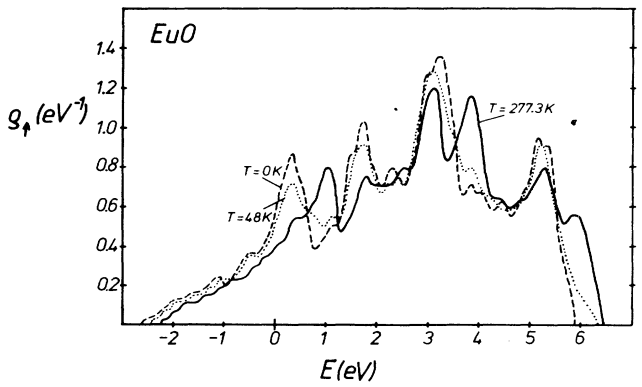

FIG. 4. Total quasiparticle density of states $\rho_\uparrow$ per atom as a function of energy for EuO at three different temperatures.

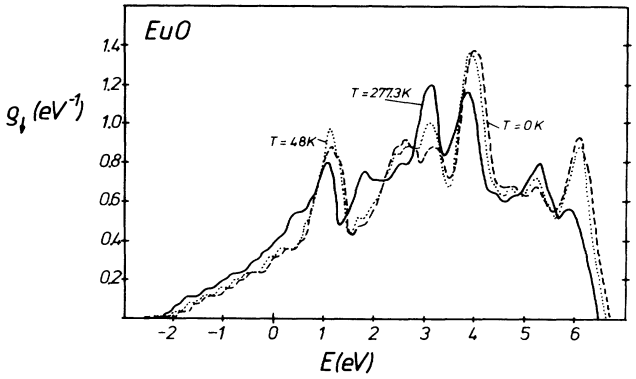

FIG. 5. The same as in Fig. 4, but for $\rho_\downarrow$.

many-body effects influence the quasiparticle energy spectrum of a ferromagnetic $4f$ system like EuO. An interesting detail is the double-peak structure of the paramagnetic Q-DOS of the $m=3$ and $m=5$ subband. In the ferromagnetic phase the lower peak of $\rho_\uparrow^{(3,5)}$ increases at cost of the upper peak, and vice versa for $\rho_\downarrow^{(3,5)}$.

A quantity, which should be directly observable in an inverse photoemission experiment, is the one-electron spectral density[29] (37). In our previous paper (I) we have discussed this function at length for the exactly solvable $T=0$ limiting case. Let us therefore concentrate ourselves here mainly on the temperature dependence. Figure 7 presents some examples for the $m=1$ subband. The $\mathbf{k}$ vectors are again chosen representatively from the ΓL direction. The $\mathbf{k}$ dependence of $A_{\mathbf{k}\sigma}^{(m)}(E)$ is, strictly speaking, an $\varepsilon_m(\mathbf{k})$ dependence. The $\varepsilon_m(\mathbf{k})$ values are indicated in Fig. 7 as small arrows. In the ferromagnetic saturation ($T=0$) $A_{\mathbf{k}\uparrow}^{(m)}$ is a trivial δ function at the energy $[\varepsilon_m(\mathbf{k})-\frac{1}{2}gS]$, corresponding to a bound state, i.e., a quasiparticle with infinite lifetime. A spin-up electron cannot exchange its spin with the completely parallel aligned f-spin system. Many-body effects are to be seen at $T=0$ only in the spin-down spectrum, because a spin-down electron can exchange its spin with the f moments, e.g., by magnon emission. A spin flip by magnon emission can of course only happen, when there are spin-up states within reach, onto which the original spin-down electrons can be scattered. This is the reason, why $A_{\mathbf{k}\downarrow}^{(m)}(E)$ is exactly in the same energy region different from zero as $\rho_\uparrow^{(m)}(E)$. In addition to this scattering part,[4] there sometimes appears in $A_{\mathbf{k}\downarrow}(E)$ a sharp δ function at higher energies, representing an infinitely living quasiparticle ("bound state"[8-11]). This quasiparticle solution, which we called in I the "polaron peak", belongs to an energy outside the region $\rho_\uparrow^{(m)} \neq 0$, so that spin flip by magnon emission is excluded. In some situations this polaron peak is pushed into the scattering part [see Figs. 4–8 in I], getting therewith a finite width. The width is broader the greater the spin-flip scattering probability, i.e., the larger the state density $\rho_\uparrow^{(m)}$ at this energy. Magnon emission of a spin-down electron is, in principle, equivalent to magnon-absorption of a spin-up electron. The latter is, however, impossible at $T=0$, since the system does not contain any magnon. This is the reason

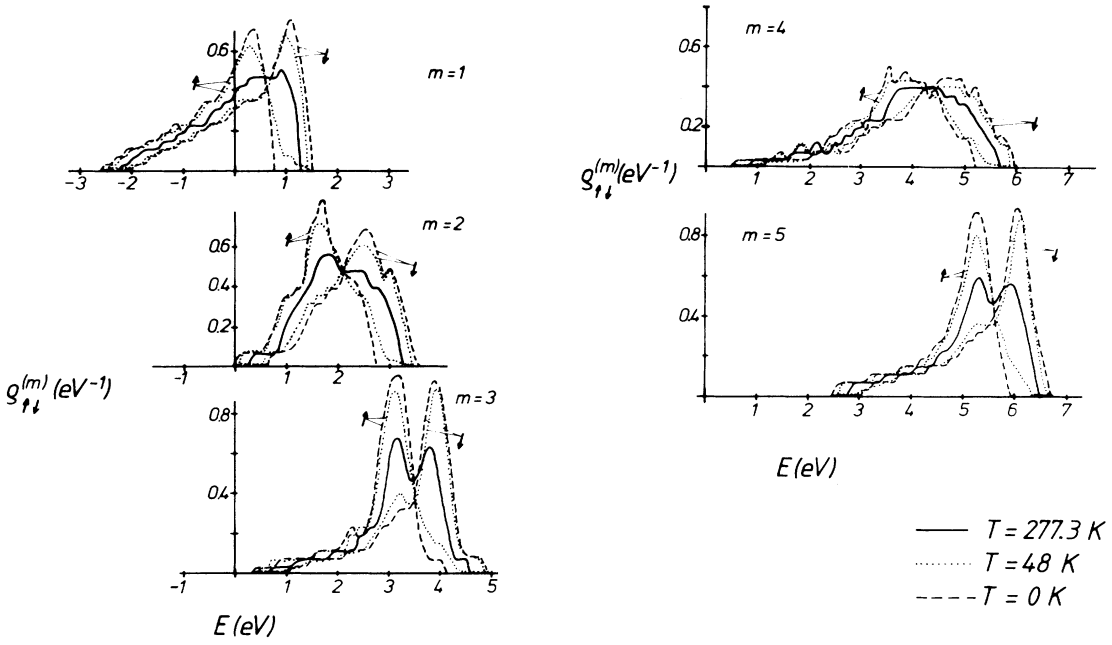

FIG. 6. Partial quasiparticle densities of states $\rho_\sigma^{(m)}$ ($m = 1,2, \ldots, 5$) of the five $5d$-subbands of EuO as function of energy E, and that for three different temperatures $T = 277.3$ K (solid line), $T = 48$ K (dotted line), and $T = 0$ K (dashed line).

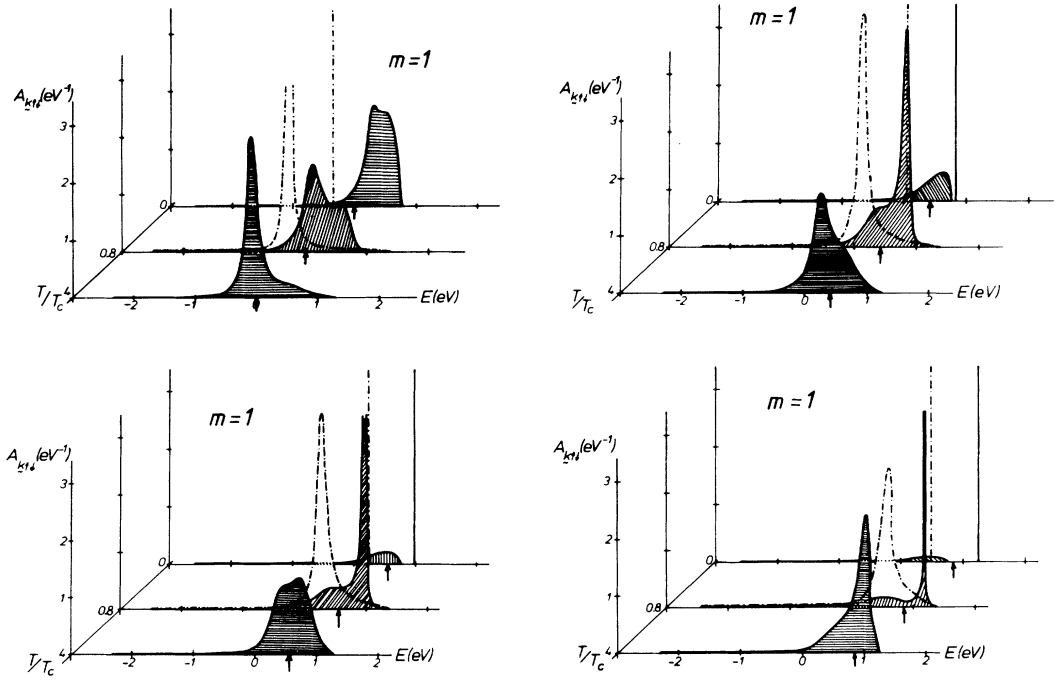

FIG. 7. One-electron spectral densities $A_{\mathbf{k}\uparrow}$ and $A_{\mathbf{k}\downarrow}$ for the $m = 1$ subband as functions of energy for three different temperatures. Solid lines for $A_{\mathbf{k}\downarrow}$; dashed-dotted lines for $A_{\mathbf{k}\uparrow}$. The four partial figures belong to four different $\mathbf{k}$ values along the ΓL direction. The corresponding Bloch energies $\varepsilon_1(\mathbf{k})$ are indicated by small arrows.

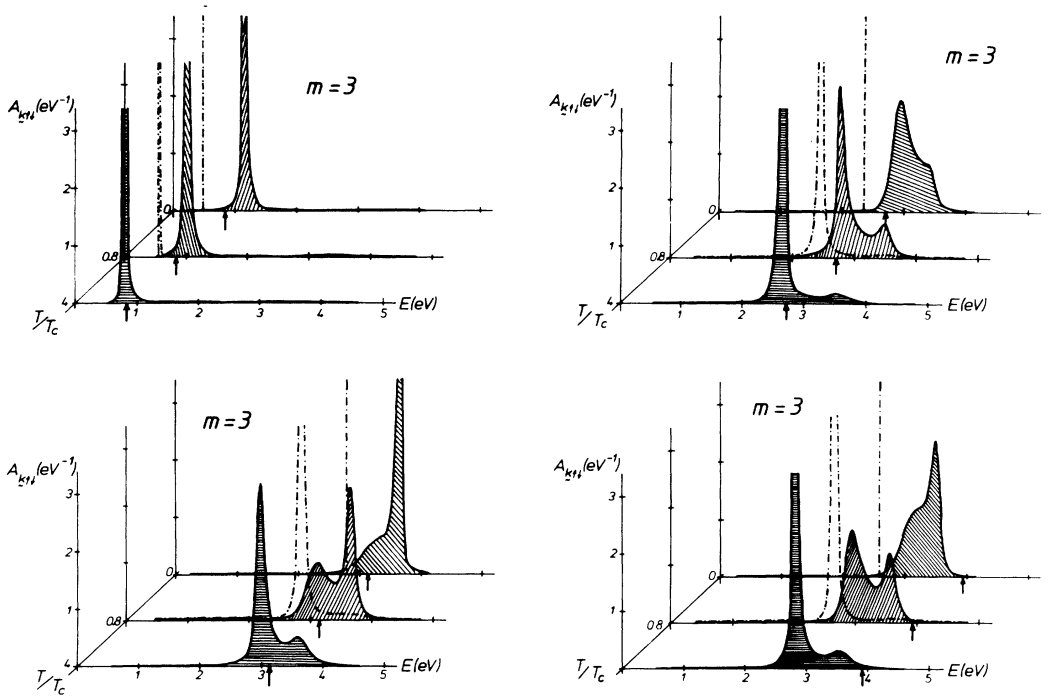

FIG. 8. The same as in Fig. 7, but for the $m = 3$ subband.

why at $T = 0$ the spin-up spectrum is so much simpler than the spin-down spectrum. At finite temperatures, however, the situation changes drastically. Examples for $T = 0.8T_c$ and $T = 4T_c$ are plotted in Figs. 7 and 8. The first observation is that bound states no longer appear. All quasiparticles have finite lifetimes. We have seen in connection with Eq. (42) that both Q-DOS $\rho_{\sigma}^{(m)}(E)$ and $\rho_{-\sigma}^{(m)}(E)$ occupy exactly the same energy regions. If a σ electron is excited into one of the quasiparticle subbands, it has therefore always the possibility to flip its spin by magnon emission or absorption. This leads to a continuum of scattering states, which coincides exactly with the

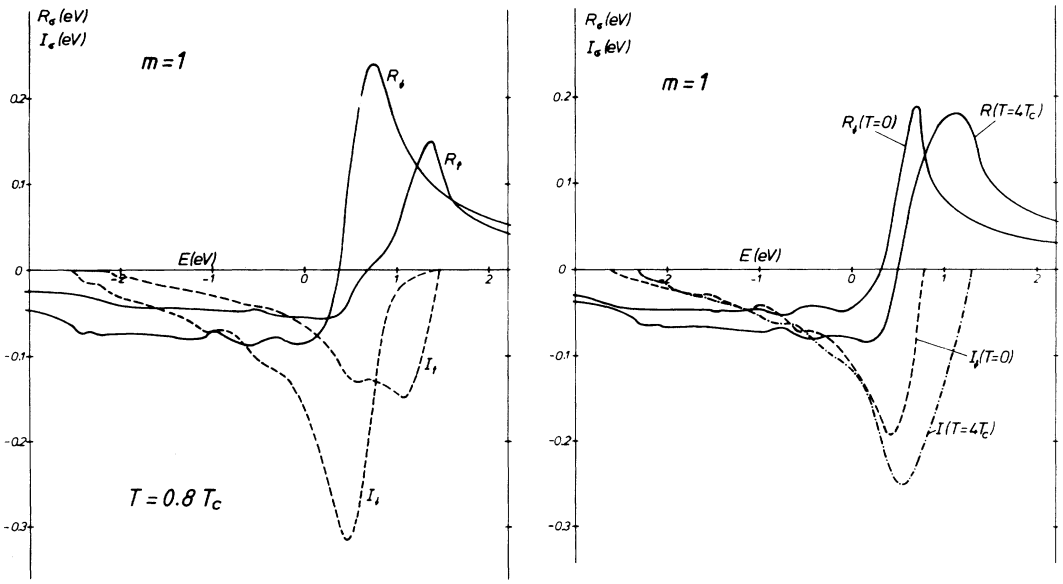

FIG. 9. Real part $R_{\sigma}^{(1)}$ (solid lines) and imaginary part $I_{\sigma}^{(1)}$ (dashed and dashed-dotted lines) of the electronic self-energy as a function of E for three different temperatures and both spin directions. The curves are calculated for the $m = 1$ subband.

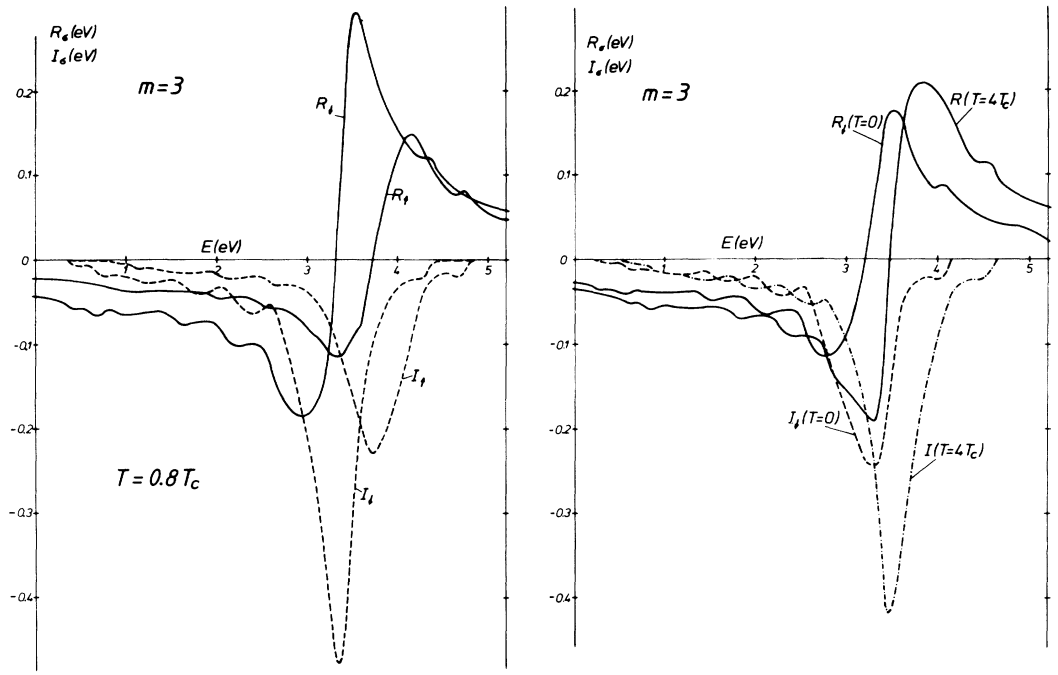

FIG. 10. The same as Fig. 9, but for the $m=3$ subband.

Q-DOS $\rho_\sigma^{(m)}$ and $\rho_{-\sigma}^{(m)}$. Although $A_{\mathbf{k}\sigma}^{(m)}$ is finite over a width of several eV, substantial spectral weight is concentrated in a relatively small region, only. The original $T=0$ polaron peak is now more or less smeared out. The polaron decay happens of course also via magnon emission or absorption. Particularly for the $m=3$ subband (Fig. 8), and similarly for the $m=5$ subband, which is not plotted, we observe in some cases interesting double-peak structures of the one-electron spectral density. One is due to a sharp bunching of the ever existing scattering states, the other to the magnetic polaron. Only the latter is a real quasiparticle with an energy $E_{m\sigma}(\mathbf{k})$ corresponding to a pole of the one-electron Green function (16):

$$E_{m\sigma}(\mathbf{k})=\varepsilon_m(\mathbf{k})-\tfrac{1}{2}gz_\sigma\langle S^z\rangle+M_\sigma^{(m)}[E_{m\sigma}(\mathbf{k})]\ . \qquad (73)$$

Experimentally it is of course not distinguishable, whether the peak in $A_{\mathbf{k}\sigma}^{(m)}$ stems from sharply bunched scattering states or from a quasiparticle in the classical sense. Summing up these spectral densities over all wave vectors of the first Brillouin zone results in the partial Q-DOS $\rho_\sigma^{(m)}$ plotted in Fig. 6.

Examples for the real and the imaginary part of the electronic self-energy $R_\sigma^{(m)}(E)$ and $I_\sigma^{(m)}(E)$ are plotted in Fig. 9 for the $m=1$ subband and in Fig. 10 for the $m=3$ subband. According to formula (42) $I_\sigma^{(m)}$ has a similar shape as $\rho_{-\sigma}^{(m)}$, since the spin-flip scattering probability of the original σ electron is higher the more $(-\sigma)$ states are available.

Our detailed results for the spectral densities $A_{\mathbf{k}\sigma}^{(m)}$ permit the derivation of temperature-dependent quasiparticle band structures, which are plotted for three different temperatures in Figs. 11–13. Figure 11 repeats for comparison the exact $T=0$ results being discussed in detail in I. The spin-up spectrum is identical to the results of the

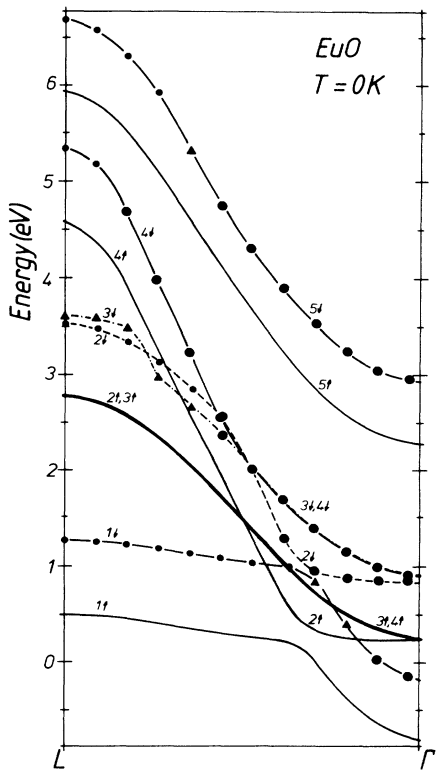

FIG. 11. Full quasiparticle band structure for EuO at $T=0$ K along the ΓL direction. Solid lines belong to spin-up quasiparticles, which have always infinite lifetimes ("bound states"). Small solid circles characterizes spin-down quasiparticles with infinite lifetimes, large solid circles correspond to well-defined quasiparticles, but with finite lifetimes, and triangles represent not well-defined quasiparticles.

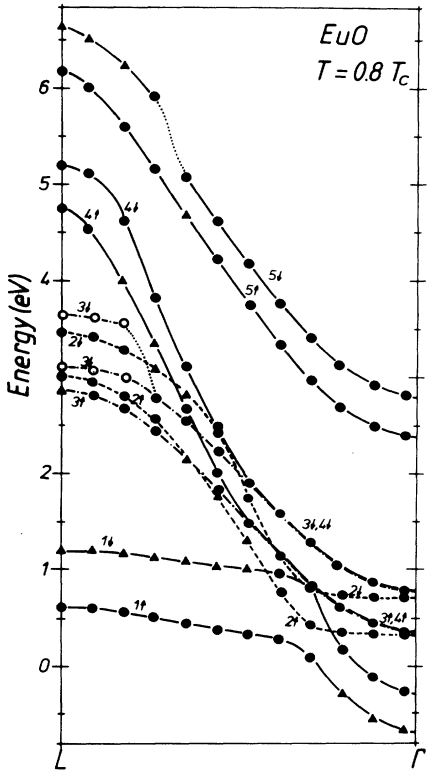

FIG. 12. Full quasiparticle band structure for EuO at $T=0.8T_c$ ($T_c=69.33$ K) in the ΓL direction. Solid circles mark well-defined quasiparticles with finite lifetimes (sharp peak in the spectral density), triangles indicate non-well-defined quasiparticles (broad peak in the spectral density). Open circles belong to a "quasiparticle splitting" according to a double-peak structure of the corresponding spectral density (see Figs. 7 and 8).

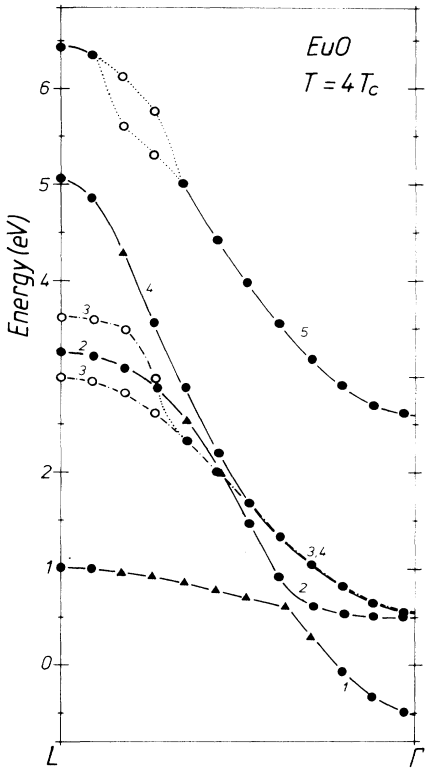

FIG. 13. The same as in Fig. 12, but for $T=4T_c$ (paramagnetic region).

self-consistent spin-polarized band calculation based on density-functional theory as described in Sec. IV of paper I. It consists, as explained above, of bound states, only, and serves as reference scheme for the one-particle spectrum $\varepsilon_m(\mathbf{k})$.

For finite temperatures ($0.8T_c$ in Fig. 12; $4T_c$ in Fig. 13) the "quasiparticle" energies, which are used in Figs. 12 and 13 for constructing the dispersion curves, are identified with the peak positions of the corresponding spectral density. We observe for $T<T_c$ an exchange splitting of each m dispersion, being roughly proportional to $g\langle S^z\rangle$. For $T>T_c$ spin-up and spin-down curves of course coincide, but nevertheless there remains a temperature dependence, now determined by the transverse spin correlation function of the f system. The striking double peak structure of the spectral density, particularly observed in parts of the $m=3$ and $m=5$ subbands, manifests itself in a "quasiparticle splitting," indicated by the open circles in Figs. 12 and 13. Let us finally point out once more, that for $T>0$ the spectra do not contain any bound state, all quasiparticles have finite lifetimes.

IV. SUMMARY

We have presented in this paper a theory for the temperature dependence of the electronic quasiparticle spectrum of ferromagnetic $4f$ systems, which has been evaluated for the insulator EuO. We used a d-f exchange model, which has been exactly solved in our previous paper I for $T=0$. We performed a self-consistent spin-polarized band-structure calculation based on density-functional theory in order to fix the one-particle Bloch energies in the d-f model as realistic as possible taking therewith into account all interactions which are not directly covered by the d-f model. We found that the d-f exchange interaction produces a strong temperature dependence, which we discussed in connection with the spectral density, the real and the imaginary part of the electronic self-energy, as well as the quasiparticle density of states. The temperature influence is in first order due to the magnetization, and in second order due to the transverse correlation function of the localized $4f$ spins. We constructed a temperature-dependent quasiparticle band structure for the ΓL direction in that part of the spectrum which has mainly $5d$ character representing the empty conduction band of the semiconductor EuO.

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