# Spin-filter effect of the europium chalcogenides: An exactly solved many-body model

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A model Hamiltonian is introduced which considers the main features of the experimental spin-filter situation such as $s$-$f$ interaction, planar geometry, and the strong external electric field. The proposed many-body model can be solved analytically and exactly using Green functions. The spin polarization of the field-emitted electrons is expressed in terms of spin-flip probabilities, which are put down to the exactly known dynamic quantities of the system. The calculated electron spin polarization shows remarkable dependencies on the electron velocity perpendicular to the emitting plane and the strength of $s$-$f$ coupling. Experimentally observed polarization values of about 90% are well understood within the framework of the proposed model. [S0163-1829(98)08137-5]

## I. INTRODUCTION

Because of their extraordinary magnetic, optic, and transport properties magnetic semiconductors, among which are the europium chalcogenides, have been the subject of numerous experimental and theoretical investigations.[1,2] Many of them focused on the spin-filter effect (SFE) of the europium chalcogenides.

The spin-filter experiment can be arranged as a field emission experiment. Here a cooled tungsten emitter is exposed to a strong stationary electrical field bending down the vacuum level of the electric potential outside the emitter. The so formed potential barrier can quantum mechanically be penetrated by the conduction band electrons of the emitter metal. The probability for this tunneling process is known to depend exponentially on the barriers height. This strong dependence can be used to obtain a ''spin filter'' by covering the original emitter with a layer of a ferromagnetically ordered material, e.g., a ferromagnetic semiconductor[3] such as EuS that makes the barrier spin dependent.

From an experimental point of view the generation of highly polarized electron beams became more and more interesting with the growing importance of the spin polarized electron spectroscopies which are presently a powerful tool in the field of analyzing magnetic properties of surfaces and thin films.[4–6] The spin-filter effect of the europium chalcogenides allows for polarization values of about 90%.[3,7–9]

Examining the SFE theoretically is worthwhile, too. Europium chalcogenides (Eu$X$, with $X=O$, S, Se, Te) show highly interesting correlation effects due to the complex interplay of itinerant conduction band electrons and localized $4f$ electrons, the latter carrying a strong magnetic moment. The so called $s$-$f$ model

$$H=H_s+H_{sf}=\sum_{ij\sigma} T_{ij}c^+_{i\sigma}c_{j\sigma}-\frac{J}{\hbar}\sum_i \boldsymbol{\sigma}_i\cdot\mathbf{S}_i \tag{1}$$

describes the interaction of both electron groups quite successfully.[10,11] $c^{(+)}_{i\sigma}$ are the usual annihilation (creation) operators for conduction band electrons with spin $\sigma$ at site $\mathbf{R}_i$. The spin of a conduction band electron at site $\mathbf{R}_i$ is denoted by $\boldsymbol{\sigma}_i$ and $\mathbf{S}_i$ represents the spin of the half filled $4f$ shell at this site. (The notation is conventional.)

The simplest possible approximation to solve the corresponding many-body problem is the mean field approximation of Eq. (1)

$$H^{\mathrm{MF}}=\sum_{ij\sigma} T_{ij}c^+_{i\sigma}c_{j\sigma}-\frac{1}{2}J\langle S^z\rangle\sum_{i,\sigma} z_\sigma n_{i\sigma}$$
$$=\sum_{ij\sigma}\left(T_{ij}-\frac{z_\sigma}{2}J\langle S^z\rangle\delta_{ij}\right)c^+_{i\sigma}c_{j\sigma} \tag{2}$$

($z_\uparrow=+1$, $z_\downarrow=-1$) which has often been used to discuss the spin-filter experiment, too.[7–9,12] The mean-field decoupled $s$-$f$ interaction term spin dependently renormalizes the one-particle energies of the free conduction band electrons (see Fig. 1), giving them an explicit spin and temperature dependence.

Below $T_c$ the conduction band splits due to the interaction of conduction band and magnetically ordering $4f$ spin lattice into two completely spin-polarized subbands. This splitting is temperature dependent and at $T=0$ of the order of $JS\approx 1$ eV. For the spin-filter experiment this would mean that below $T_c$ only $\sigma=\uparrow$ electrons could be emitted, as the subband for $\sigma=\downarrow$ electrons lies much higher than the $\sigma=\uparrow$ subband and $\downarrow$ electrons ''see'' accordingly a much higher tunnel barrier.

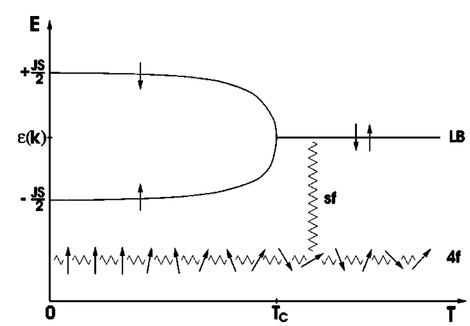


FIG. 1. Temperature-dependent quasiparticle band structure of the $s$-$f$ model in the mean-field approximation (schematically).

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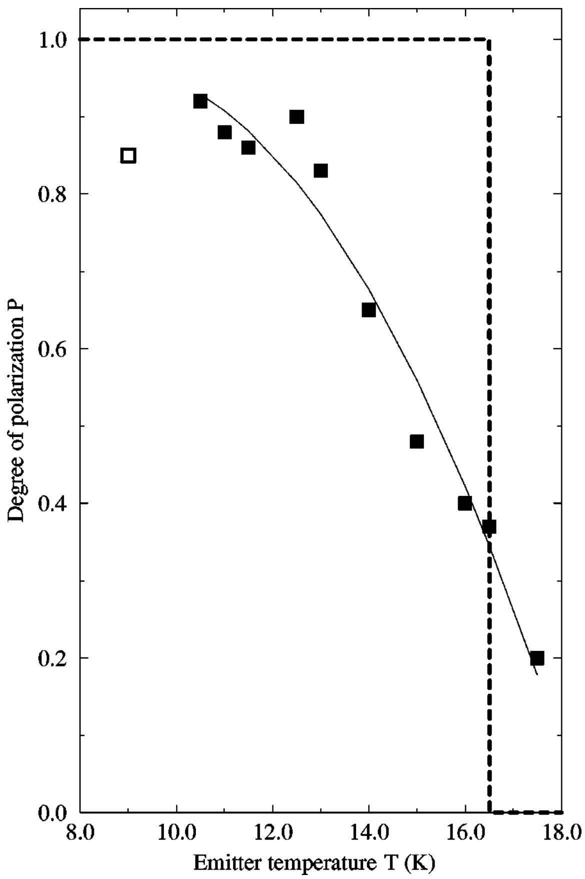


FIG. 2. The temperature-dependent degree of polarization for field emitted electrons in a spin-filter experiment. The dotted line is the prediction of the often used mean-field solution for the $s$-$f$ model. Data were taken from Kisker *et al.* (Ref. 9), the point ($T = 9$ K, $P = 85\%$) was taken from Ref. 8.

The mean field picture thus predicts a degree of polarization for the emitted electrons that should be very close to 100% for all temperatures below $T_c$ and 0% above. However, this does not agree very well with the experimental data (see Fig. 2).[9] The main failure of the mean field approximation is probably the complete suppression of spin-flip processes.

Knowledge about the $s$-$f$ model has increased[2,13–17] since the first attempts of applying it to the SFE in the early 1970's.[12,7,18] The aim of the present paper is a new interpretation of the SFE based on recent progress which permits us to treat the many-body problem of the spin-filter effect, including the external electric field, exactly.

## II. ELECTRON SPIN POLARIZATION

### A. Polarization and probabilities

In this section it will be shown how the central quantity of the spin-filter experiment, the polarization, can be connected with the dynamic quantities of the system, the Green functions, which will be determined in the following section from the many-body model. The vector spin polarization **P** of an ensemble of electrons is defined as the expectation value of the Pauli spin matrices. It is easiest to handle its projection on the preferential direction of spins, the scalar quantity $P$ (degree of polarization),

$$P \overset{\text{def}}{=} \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}, \tag{3}$$

where $N_\uparrow$ is the number of electrons with spin $\sigma = \uparrow$ and $N_\downarrow$ the number of electrons with spin $\sigma = \downarrow$. We now consider the probabilities for electrons with original spin $\sigma$ to flip their spin, i.e., the flip probabilities $p_\sigma$. If, for example, the originally prepared state was $\downarrow$, then $p_\downarrow$ gives the probability to measure an electron in the $\uparrow$ state.

Assuming an unpolarized beam of electrons ($N_{0\uparrow} = N_{0\downarrow}$) passing through a spin-filter box we obtain very easily the polarization of the out-coming beam using Eq. (3) and the flip probabilities $p_\sigma$ which are completely determined by the physical properties of the spin-filter box:

$$N_\uparrow = N_{0\uparrow}(1 - p_\uparrow) + N_{0\downarrow} p_\downarrow = \frac{N_0}{2}(1 + p_\downarrow - p_\uparrow), \tag{4}$$

$$N_\downarrow = N_{0\downarrow}(1 - p_\downarrow) + N_{0\uparrow} p_\uparrow = \frac{N_0}{2}[1 - (p_\downarrow - p_\uparrow)], \tag{5}$$

$$P = \frac{(N_0/2)[1 + p_{\text{eff}} - (1 - p_{eff})]}{N_0} = p_{\text{eff}}. \tag{6}$$

Here we introduced $p_{\text{eff}} \overset{\text{def}}{=} p_\downarrow - p_\uparrow$, the effective flip ratio of the spin filter. Ask for the polarization, we should thus try to get the flip probabilities from a theoretical model, i.e., Green functions.

### B. Probabilities and Green functions

Let us consider the following example: What is the (non-flip) probability $\overline{p(t)}$ to measure at time $t$ an electron with wave vector **k**, if at $t = 0$ an electron in this state had been prepared? The answer is given[19] by the overlap of initial state $c_{\mathbf{k}}^+(0)|0\rangle$ and final state $c_{\mathbf{k}}^+(t)|0\rangle$. $c_{\mathbf{k}}^{(+)}(t)$ (creates) annihilates an electron at time $t$ with wave vector **k**. The state $|0\rangle$ is the electron and magnon vacuum:

$$\overline{p(t)} = |\langle 0| c_{\mathbf{k}}(t) c_{\mathbf{k}}^+(0)|0\rangle|^2. \tag{7}$$

One sees the similarity of the probability $\overline{p(t)}$ with the well-known entity of many-body theory, the time-dependent spectral density of the one-electron Green function:

$$S_{\mathbf{k}}(t,0) = \frac{1}{2\pi}\langle [c_{\mathbf{k}}(t), c_{\mathbf{k}}^+(0)]_+\rangle. \tag{8}$$

In our special case ($T = 0$, $n = 0$), the average denoted by the angular brackets has to be taken with the $|0\rangle$ state, i.e., with the electron and magnon vacuum. Therefore one of the terms in the anticommutator does not contribute.

Spectral density (8) and Green function $G_{\mathbf{k}\sigma}(E) \equiv \langle\langle c_{\mathbf{k}\sigma}; c_{\mathbf{k}\sigma}^+\rangle\rangle_E$ are closely related. Both will be determined in Sec. IV. From Eqs. (7) and (8) we obtain immediately

$$\overline{p(t)} = 4\pi^2 |S_{\mathbf{k}}(t)|^2. \tag{9}$$

### III. THEORETICAL MODEL

The aim of this section is to develop a many-body model of the spin filter which incorporates the main features of the experimental situation. We make the following two assumptions which allow us to treat the corresponding many-body problem exactly:

(1) The tunneling processes of the emitted electrons are independent from each other; i.e., the conduction band is nearly empty $(n=0)$.
(2) The $4f$ lattice is ferromagnetically saturated, i.e., low temperatures $(T=0)$.

#### A. Geometry

Our calculations are done for a *planar* spin filter, i.e., a sandwichlike batch of monolayers which are translational invariant parallel to their plane. This matches the experimental situation (field emission through a EuS layer) and provides at the same time the proper symmetry to include the influence of the strong electric field.

The treatment of a planar system is based on the decomposition of the whole system into $n$ equivalent two-dimensional sublattices (atomic layers) with $N_s$ lattice points each:

$$\mathbf{R}_{i\alpha}=\mathbf{R}_i+\mathbf{r}_\alpha . \tag{10}$$

$\mathbf{R}_i$ and $\mathbf{r}_\alpha$ are perpendicular to each other. $\mathbf{r}_\alpha$ points to the atomic layer with index $\alpha$, whereas $\mathbf{R}_i$ points towards the lattice point with index $i$ inside this layer.

From the lattice vector $\mathbf{R}_{i\alpha}$ this subscription is carried on to *all* operators and derived quantities; greek indices generally refer to the layer while latin indices refer to lattice points within this layer:

$$O_i \rightarrow O_{i\alpha}, \quad O_{ij}\rightarrow O_{ij}^{\alpha\beta}, \quad O_{ikj}\rightarrow O_{ikj}^{\alpha\beta\gamma}. \tag{11}$$

Fourier transformation into $\mathbf{k}$ space is reasonably defined only within the two-dimensional sublattices, which are still invariant under translation

$$O_{i\alpha}=\frac{1}{\sqrt{N_s}}\sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{R}_i}O_{\mathbf{k}\alpha}, \tag{12}$$

$$O_{\mathbf{k}\alpha}=\frac{1}{\sqrt{N_s}}\sum_{i} e^{-i\mathbf{k}\mathbf{R}_i}O_{i\alpha}. \tag{13}$$

$\mathbf{k}$ means in all of the following considerations a vector of the two-dimensional Brillouin-zone (BZ) of one layer.

#### B. $s$-$f$ interaction

It is convenient to write Eq. (1) in a more suitable form for our purposes:

$$H_{sf}=-\frac{1}{2}J\sum_{i\alpha\sigma}(z_\sigma S_{i\alpha}^z n_{i\alpha\sigma}+S_{i\alpha}^\sigma c_{i\alpha-\sigma}^+ c_{i\alpha\sigma}). \tag{14}$$

Here the spin operators for the conduction electrons are expressed in terms of the creation and annihilation operators $c_{i\alpha\sigma}^{(+)}$:

$$\frac{1}{\hbar}\sigma_{i\alpha}^+=c_{i\alpha\uparrow}^+c_{i\alpha\downarrow}, \quad \frac{1}{\hbar}\sigma_{i\alpha}^-=c_{i\alpha\downarrow}^+c_{i\alpha\uparrow}, \tag{15}$$

$$\frac{1}{\hbar}\sigma_{i\alpha}^z=\frac{1}{2}\sum_\sigma z_\sigma n_{i\alpha\sigma}, \tag{16}$$

with $z_\uparrow=+1$, $z_\downarrow=-1$ and where the identity for the ladder operators

$$S_{i\alpha}^{\uparrow(\downarrow)}\equiv S_{i\alpha}^{\pm}=S_{i\alpha}^x \pm iS_{i\alpha}^y \tag{17}$$

has been used.

This representation already indicates some physics: The first term in Eq. (14) describes the interaction of the $z$ components of the spins similar to the well-known Ising model.[20] Accordingly it will be called the Ising term. The second term in Eq. (14) is nondiagonal in spin indices and thus is responsible for spin-flip processes; it will be referred to as the spin-flip term.

Interactions among the strongly localized $4f$ spins might be taken into account via a Heisenberg term,[21] but will here be neglected, as we are mainly interested in the situation of conduction band electrons. Magnon energies are two to three orders of magnitude smaller than the other energy scales of the system such as bandwidth or $s$-$f$ coupling.

For similar reasons the interaction among different conduction band electrons will not be part of the model: europium chalcogenides are magnetic semiconductors, ordering at fairly low temperatures [$T_c^{\mathrm{EuS}}=16.57$ K (Ref. 1)]. In the range of temperatures that is of interest to us, the conduction band is nearly empty, and thus the contribution of electron-electron interaction to the total energy of the system will be negligible.

#### C. External electric field

The Hamiltonian of an external electric field

$$H_V=-\hat{\mathbf{P}}\cdot\mathbf{F} \tag{18}$$

is a one-particle operator. Rewriting it in terms of second quantization

$$H_V=\sum_n h_V^{(n)}=\sum_{\substack{ij\sigma\\ \alpha\beta}} M_{ij}^{\alpha\beta}c_{i\alpha\sigma}^+c_{j\beta\sigma}, \tag{19}$$

we have to determine the matrix elements $M_{ij}^{\alpha\beta}$. $h_V^{(n)}$ acts in the one-particle-Hilbert space of the $n$th electron; $|i\alpha\rangle$ are elements of a complete orthonormal basis, for instance, Wannier states.

Calculating $M_{ij}^{\alpha\beta}$, we have to specify the vector of electric field $\mathbf{F}$ and the operator of the electric dipole momentum $\hat{\mathbf{P}}$. The electric field is assumed to act homogeneously along the $z$ axis, i.e., perpendicular to the Eu$X$ film (see Fig. 3):

$$\mathbf{F}=(F_x,F_x,F_z)=(0,0,-f=\mathrm{const}). \tag{20}$$

With

$$\hat{\mathbf{P}}=-\mathrm{e}\sum_n \hat{\mathbf{r}}^{(n)}, \tag{21}$$

we evaluate the matrix elements

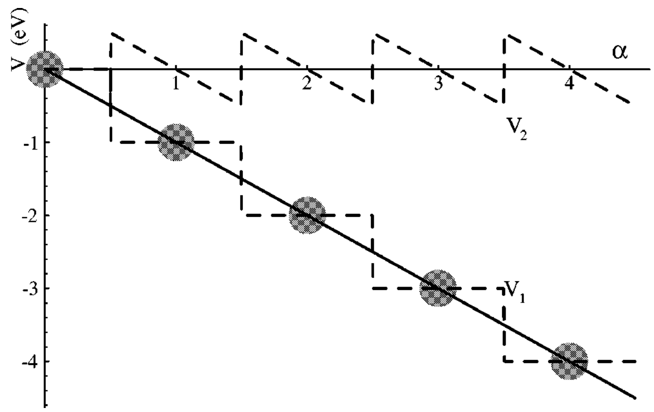


FIG. 3. Decomposition of a linear potential into a steplike ($V_1$) and saw-tooth-like part. The points mark the field displaced centers of gravity of the conduction band in the layers. $\alpha$ is the layer index.

$$M_{ij}^{\alpha\beta}=-ef\langle j\beta|(\hat{\mathbf{r}})_z|i\alpha\rangle\cong-ef(\mathbf{R}_{i\alpha})_z\delta_{ij}^{\alpha\beta}$$
$$=-ef\alpha a_0\delta_{ij}^{\alpha\beta}=-\alpha u\,\delta_{ij}^{\alpha\beta}. \qquad (22)$$

Here we assumed the Wannier functions to be eigenfunctions of the position-space operator, which should hold in good approximation. Additionally we used $(\mathbf{R}_{i\alpha})_z\equiv|\mathbf{r}_\alpha|=\alpha a_0$: the $z$ component of lattice vector $\mathbf{R}_{i\alpha}$ equals the product of layer index $\alpha$ and lattice constant $a_0$. Furthermore we introduced the interlayer potential difference $u=efa_0$.

For the Hamiltonian of a homogeneous field, acting along the $z$ axis, i.e., perpendicular to spin filtering Eu$X$ film we eventually obtain

$$H_V=-u\sum_{i\alpha\sigma}\alpha n_{i\alpha\sigma}. \qquad (23)$$

Finally, we propose the following model Hamiltonian for the spin filter:

$$H=H_s+H_{sf}+H_V. \qquad (24)$$

## IV. SOLUTION OF THE MANY-BODY PROBLEM

### A. *s-f* model for $T=0$, $n=0$

The theoretical model developed in the previous section will now be solved. We consider a single test electron in the otherwise empty conduction band and a ferromagnetic saturated $4f$-spin system. This special case of the $s$-$f$ model is not only fundamental for the understanding of the spin-filter effect as it meets the experimental conditions, it can also be solved exactly,[22,16] even for the planar geometry.[23]

The retarded one electron anticommutator-Green function

$$G_{ij\sigma}^{\alpha\beta}(E)=\langle\langle c_{i\alpha\sigma};c_{j\beta\sigma}^{+}\rangle\rangle_E \qquad (25)$$

will give us, among other interesting information, the time-dependent spectral density, which is needed for calculating the flip-probabilities (9) and the polarization of the emitted electrons (6):

$$S_{\mathbf{k}\sigma}^{\alpha\beta}(t)=\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty}dE e^{-(i/\hbar)Et}S_{\mathbf{k}\sigma}^{\alpha\beta}(E), \qquad (26)$$

$$S_{\mathbf{k}\sigma}^{\alpha\beta}(E)=-\frac{1}{\pi}\,\mathrm{Im}\{G_{\mathbf{k}\sigma}^{\alpha\beta}(E+i0^+)\}. \qquad (27)$$

To determine this Green function, one has to solve its equation of motion

$$EG_{ij\sigma}^{\alpha\beta}(E)=\hbar\langle[c_{i\alpha\sigma},c_{j\beta\sigma}^{+}]_+\rangle+\langle\langle[c_{i\alpha\sigma},H]_-;c_{j\beta\sigma}^{+}\rangle\rangle_E. \qquad (28)$$

The higher Green functions, appearing on the right-hand side of Eq. (28)

$$\Gamma_{ik,j\sigma}^{\alpha\gamma\beta}(E)=\langle\langle S_{i\alpha}^{z}c_{k\gamma\sigma};c_{j\beta\sigma}^{+}\rangle\rangle_E, \qquad (29)$$

$$F_{ik,j\sigma}^{\alpha\gamma\beta}(E))=\langle\langle S_{i\alpha}^{-\sigma}c_{k\gamma-\sigma};c_{j\beta\sigma}^{+}\rangle\rangle_E, \qquad (30)$$

are to be calculated by solving *their* equations of motion. This procedure usually leads to an infinite hierarchy of coupled Green functions and their equations of motion. To get any solution, physically reasonable decouplings are needed. One possible treatment would be the mean field approximation where function (29) can be expressed in terms of function (25) and function (30) is suppressed completely.

After doing the two-dimensional Fourier transformation parallel to the planes, the equation of motion (28) of the one-electron Green function $G_{ij\sigma}^{\alpha\beta}(E)$ reads as follows:

$$\sum_{\delta}\,[(E+\tfrac{1}{2}z_\sigma J\hbar S)\delta_{\alpha\delta}-\epsilon_{\alpha\delta}(\mathbf{k})]G_{\mathbf{k}\sigma}^{\delta\beta}$$
$$=\hbar\,\delta_{\alpha\beta}-\frac{J}{2\sqrt{N_s}}\sum_{\mathbf{q}}F_{\mathbf{kq}\sigma}^{\alpha\alpha\beta}. \qquad (31)$$

In the case of an empty conduction band ($n=0$) and ferromagnetic saturation of the $f$-spin lattice ($T=0$) which is considered here, we can solve this exactly. Writing down the equation of motion of the so-called flip function $F_{ik,j\sigma}(E)$ [Eq. (30)] one recognizes that all higher Green functions may be expressed in terms of already known ones or vanish.[24,23] We find the following expression:

$$\frac{1}{\sqrt{N_s}}\sum_{\mathbf{q}}F_{\mathbf{kq}\downarrow}^{\alpha\alpha\beta}=-\frac{J\hbar^2SB_\alpha(E)}{1-\frac{1}{2}J\hbar B_\alpha(E)}G_{\mathbf{k}\downarrow}^{\alpha\beta}, \qquad (32)$$

which expresses the flip function completely in terms of the one-electron Green function $G_{\mathbf{k}\sigma}^{\alpha\beta}(E)$. Here we introduced the complex propagator $B_\alpha(E)$,

$$B_\alpha(E)=\frac{1}{N_s}\sum_{\mathbf{q}}G_{\mathbf{q}\uparrow}^{\alpha\alpha}(E). \qquad (33)$$

Equations (32) and (31) form a coupled system of equations. The equation of motion (31) is at this point obviously equivalent to a matrix multiplication which may be written in the following compact formulation:

$$(\mathbf{E}-\mathbf{H}_{\mathbf{k}\sigma})\cdot\mathbf{G}_{\mathbf{k}\sigma}=\hbar\mathbf{I}. \qquad (34)$$

$\mathbf{H}_{\mathbf{k}\sigma}$ is the effective Hamiltonian of the one-dimensional problem of an atomic chain perpendicular to the translational invariant layers. In site representation it reads

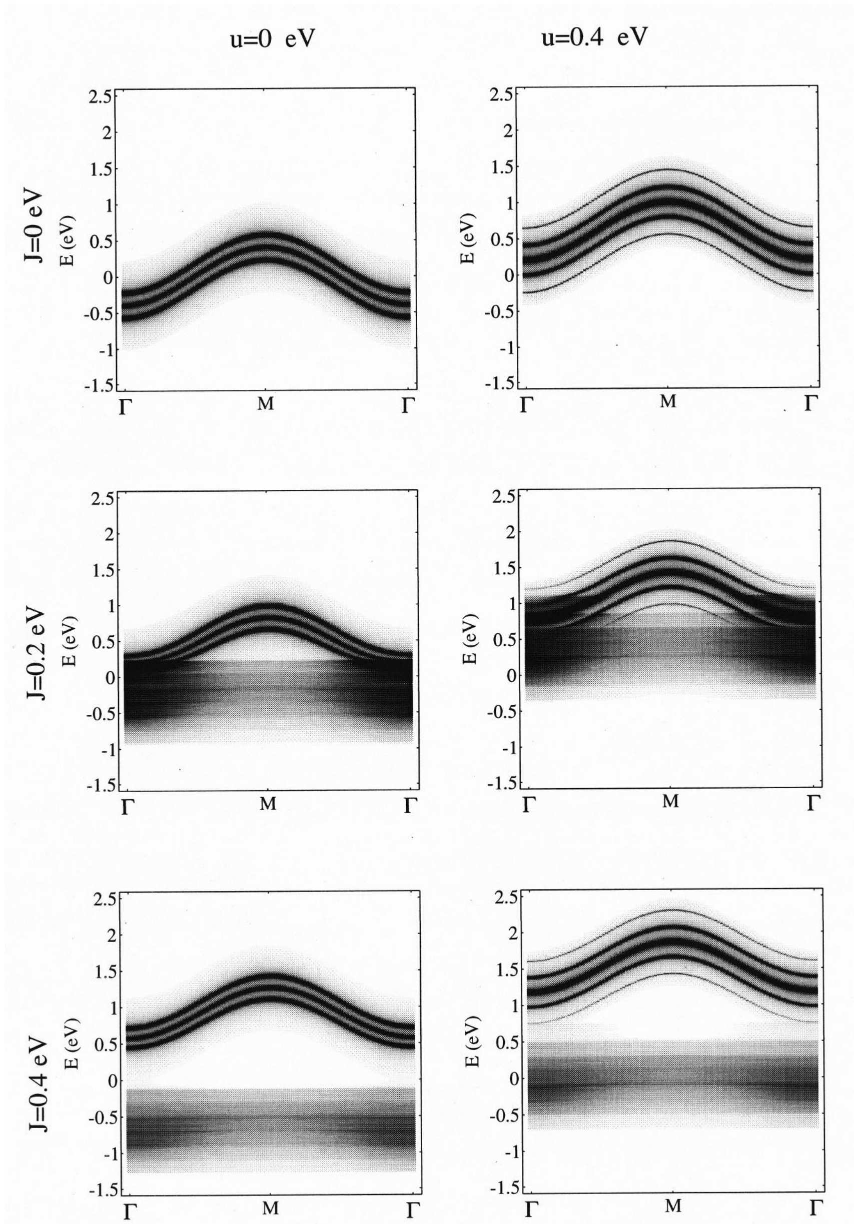


FIG. 4. Density plot of the spectral densities $S_{\mathbf{k}\sigma\downarrow}$ of the middle layer of a five layer spin filter film with and without (right and left columns, respectively) external electric field for several values of coupling strength $J$ between $4f$ spins and the conduction band

$$\mathbf{H}_{\mathbf{k}\sigma}=\begin{pmatrix} a_1 & b_{12} & b_{13} & & b_{1n} \\ b_{21} & a_2 & b_{23} & \cdots & b_{2n} \\ b_{31} & b_{32} & a_3 & & b_{3n} \\ & \vdots & & \ddots & \vdots \\ b_{n1} & b_{n2} & b_{n3} & \cdots & a_n \end{pmatrix} \tag{35}$$

with its matrix elements

$$a_\alpha=\epsilon_{\alpha\alpha}(\mathbf{k})+\Sigma_\sigma^\alpha(E), \tag{36}$$

$$b_{\alpha\beta}=\epsilon_{\alpha\beta}(\mathbf{k}), \tag{37}$$

containing the complex, local, and spin-depending self-energy $\Sigma_\sigma^\alpha$

$$\Sigma_\sigma^\alpha(E)=-z_\sigma\,\tfrac{1}{2}J\hbar S\left(1+\frac{1-z_\sigma}{2}\,\frac{J\hbar B_\alpha(E)}{1-\frac{1}{2}J\hbar B_\alpha(E)}\right), \tag{38}$$

the complex propagator $B_\alpha(E)$ [Eq. (33)], and the Fourier-transformed hopping integrals $\epsilon_{\alpha\beta}(\mathbf{k})$. It should be noticed that the self-energy for $\sigma=\uparrow$ electrons is trivial. This is due to the fact, that these electrons cannot participate in the spin-flip processes, so that their interaction with the ferromagnetically saturated $4f$ spins is restricted to a rigid energy shift of the $\sigma=\uparrow$ conduction band.

The propagator $B_\alpha(E)$ and the self-energy $\Sigma_\sigma^\alpha$ are layer dependent (index $\alpha$) but independent of the in-plane wave vector $\mathbf{k}$. The latter is due to our neglect of magnon energies which is not necessary but convenient and reasonable since they are two to three orders of magnitudes smaller than other typical energy scales of the system (bandwidth, $s$-$f$ cou-

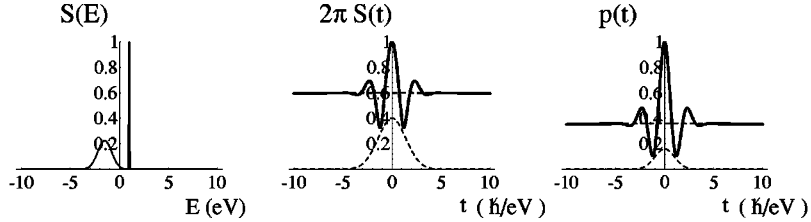


FIG. 5. The nonflip probability for electrons in the spin filter is given by the square of the time-dependent spectral density of the one-electron Green function. Shown are typical shapes of the $\sigma=\downarrow$ spectral densities of the spin-filter model: energy-dependent (left) and time-dependent (middle) and the corresponding time-dependent nonflip probability (right).

pling). However, our model might be solved exactly with full consideration of the magnon energies. From Eq. (34) we get finally the exact solution of the many-body system by matrix inversion:

$$\mathbf{G}_{\mathbf{k}\sigma}=\hbar(\mathbf{E}-\mathbf{H}_{\mathbf{k}\sigma})^{-1}. \tag{39}$$

### B. Solution with electric field

The Hamiltonian of the electric field (23) is a single-particle operator:

$$H_V=\sum_{\substack{ij\sigma\\ \alpha\beta}} M_{ij}^{\alpha\beta}c_{i\alpha\sigma}^{+}c_{j\beta\sigma}=-u\sum_{i\alpha\sigma}\alpha n_{i\alpha\sigma}. \tag{40}$$

Expressed in terms of second quantization, i.e., by means of the electron creation and annihilation operators the electric-field operator $H_V$ is therefore of the same structure as the operator of the kinetic energy of electrons $H_s$. They can be summed up:

$$H=H_s+H_V+H_{sf}=\sum_{\substack{ij\sigma\\ \alpha\beta}} \tilde{T}_{ij}^{\alpha\beta}c_{i\alpha\sigma}^{+}c_{j\beta\sigma}+H_{sf}, \tag{41}$$

$$T_{ij}^{\alpha\beta}\rightarrow\tilde{T}_{ij}^{\alpha\beta}\overset{\text{def}}{=}T_{ij}^{\alpha\beta}-\alpha u\,\delta_{ij}^{\alpha\beta}. \tag{42}$$

The renormalization of the hopping matrix elements by the external field is equivalent to a displacement of the Bloch-band centers of gravity by a position-dependent amount for each layer (see Fig. 3).

An external electric field thus renormalizes the layer-dependent self-energy

$$\Sigma_\sigma^\alpha\rightarrow\tilde{\Sigma}_\sigma^\alpha\overset{\text{def}}{=}\Sigma_\sigma^\alpha-\alpha u. \tag{43}$$

However, the principal structure of the many-body problem remains unaffected. Its solution is given by

$$\mathbf{G}_{\mathbf{k}\sigma}=\hbar(\mathbf{E}-\tilde{\mathbf{H}}_{\mathbf{k}\sigma})^{-1}, \tag{44}$$

with $\tilde{\mathbf{H}}_{\mathbf{k}\sigma}$ defined analogously to Eq. (35) with the renormalized self-energy (43).

The matrix inversion in Eq. (44) is done numerically for a simple cubic film with layers parallel to the (100) face.

## V. RESULTS

As stated above, the self-energy for $\sigma=\uparrow$ electrons is trivial. This is due to the fact that this electron group cannot participate in the spin-flip processes, so that its interaction with the ferromagnetically saturated $4f$ spins is restricted to rigid energy shift of the $\sigma=\uparrow$ conduction band. For this reason we now focus on the discussion of the $\sigma=\downarrow$ results.

### A. Spectral densities

With the Green functions given by Eq. (44) we can calculate the spectral densities $S_{\mathbf{k}\sigma}^{\alpha\alpha}$. They depend on the spin direction $\sigma$ of the test electron as well as on the layer-index $\alpha$ and the in-plane wave vector $\mathbf{k}$:

$$S_{\mathbf{k}\sigma}^{\alpha\alpha}(E)=-\frac{1}{\pi}\,\mathrm{Im}\{G_{\mathbf{k}\sigma}^{\alpha\alpha}(E+i0^{+})\}, \tag{45}$$

where $G_{\mathbf{k}\sigma}^{\alpha\alpha}$ is the element $(\mathbf{G}_{\mathbf{k}\sigma})_{\alpha\alpha}$ of the Green function matrix (44).

Figure 4 shows the spectral density $S_{\mathbf{k}\sigma\downarrow}^{3,3}$ for the center layer ($\alpha=3$) of a five-layer film with and without (right and left column, respectively) external electric field for no, medium, and strong (top, middle, bottom lines, respectively) interaction between $4f$ spins and conduction band. The top left of Fig. 4 shows the well-known dispersion of the free Bloch electron gas in the two-dimensional Brillouin zone.

As the system consists of five layers one might expect five excitation energies. However, for symmetry reasons two pairs of them are degenerated; we see only three peaks at each $\mathbf{k}$ point. By switching on an external electric field perpendicular to the film, this degeneracy is lifted and five different peaks can be observed (top right of Fig. 4).

The middle and bottom lines of Fig. 4 show the situation for finite values of the coupling strength $J$ between $4f$ spins and conduction band electrons. In each of these pictures we find two main structures: an energetically lower lying broad and dispersionless flip band and at higher energies a sharply peaked structure which corresponds to the magnetic polaron and shows a Bloch-like dispersion.

The flip band originates from spin-flip processes of the conduction band electrons. Via the $s$-$f$ interaction, the $\sigma=\downarrow$ conduction band electron can emit a magnon, i.e., it causes a spin deviation in the ferromagnetically saturated lattice of $4f$ spins. As this process is of course forbidden for $\sigma=\uparrow$ electrons, the spectral densities $S_{\mathbf{k}\sigma\uparrow}$ for $\sigma=\uparrow$ electrons are rather trivial. They are not shown separately.

The sharply peaked structure corresponds to a quasiparticle with in most cases infinite lifetime: the magnetic polaron. This means, in analogy to the ''normal'' polaron, an electron, renormalized by a cloud of virtual excitations, namely, magnons. As this quasiparticle propagates freely through the crystal lattice, the corresponding structures in the spectral densities show therefore a Bloch-like dispersion.

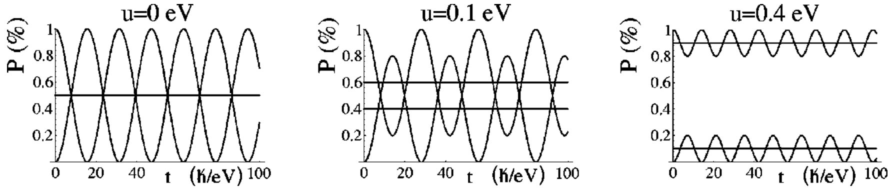


FIG. 6. Time-dependent probabilities $\overline{p}^{11}(t)$ (starting at $p=1$) and $\overline{p}^{12}(t)$ (starting at $p=0$) of finding an electron in the first or second layer at time $t$ for different values of the external field ($u$). Time is given in $\hbar/\mathrm{eV}=6.6\times10^{-16}$ sec. Straight lines are time average.

In the strong coupling regime ($J>0.2$ eV) both structures are energetically clearly separated, the polaron is represented by $\delta$ peaks and has, therefore, an infinite lifetime. This changes at weaker couplings: At $J\approx0.2$ eV, i.e., realistic values for EuS, the polaron peak touches the flip band and becomes considerably broadened near the $\Gamma$ point of the two-dimensional Brillouin zone. The lifetime of the polaron under these circumstances is finite and of the order of $1\,\hbar/eV \approx 10^{-15}$ sec.

The external electric field (right column of Fig. 4) mainly increases the energetic distances between the layers and thereby strongly influences the shape of all spectral densities. The polaronic peaks become more separated. As the flip band reproduces roughly the shape of the ($\sigma=\uparrow$) DOS, the flip band changes with the ($\sigma=\uparrow$) DOS under the influence of the electric field, too. Because of Eq. (9) one should expect a similarly significant field induced change of the transition and spin-flip probabilities. This will be investigated in the following subsection.

### B. Probabilities

We apply Eq. (9) to the typical $\sigma=\downarrow$ spectral density of the $s$-$f$ model. As calculated above [Eqs. (45), (44)] and shown in Fig. 5 it consists at each $\mathbf{k}$ point of the broad flip band, written now as $f(E)$, a continuous function of energy without singularities, and the $\delta$-like polaron band $\hbar\,\delta(E-E_0)$:

$$S(E)=\alpha_1 f(E)+\alpha_2\hbar\,\delta(E-E_0). \tag{46}$$

The $\alpha_n$ are the spectral weights ($\alpha_1+\alpha_2=1$).

From Eq. (46) one finds with Eq. (9)

$$\overline{p}(t)=|\alpha_1\tilde{f}(t)+\alpha_2 e^{-(i/\hbar)E_0 t}|^2 \tag{47}$$

because of the linearity of the Fourier transformation. With Parsevals theorem

$$\int_{-\infty}^{+\infty}|f(E)|^2 dE=\int_{-\infty}^{+\infty}|\tilde{f}(t)|^2 dt \tag{48}$$

we conclude from the normalization of $f(E)$ that $|\tilde{f}(t)|^2$ must vanish quicker than $1/t$ for $t\to\infty$.

For a typical spectral density of our model we therefore find from Eqs. (46) and (9)

$$\overline{p}(t)\xrightarrow{t\to\infty}|\alpha_2|^2. \tag{49}$$

This interesting result shows that the nonflip probability for a ($\sigma=\downarrow$) electron is completely determined by the spectral weight of the polaron peak in the spectral density and therefore strongly dependent on position in the Brillouin zone, coupling strength, and temperature.

We ask now for the probability of finding an electron independent of its spin direction in a layer with index $\beta$ at time $t$ after we prepared it at time $t=0$ in layer $\alpha$. Generalizing Eq. (9) we find

$$\overline{p}_{\mathbf{k}}^{\alpha\beta}(t)=4\pi^2|S_{\mathbf{k}}^{\alpha\beta}(t)|^2. \tag{50}$$

We will illustrate Eq. (50) by investigating it analytically for a two layer system of free electrons (i.e., $J=0$) with applied electric field. The spectral densities have a double peak structure,

$$S_{\mathbf{k}}(E)=\hbar\{\alpha_1\delta[E-E_1(\mathbf{k})]+\alpha_2\delta[E-E_2(\mathbf{k})]\}, \tag{51}$$

where the $\alpha_n$ are again the spectral weights of the $\delta$ peaks ($\alpha_1+\alpha_2=1$) and $E_n$ is the $n$th excitation energy of the system. $E_n$ is given as the $n$th pole of the Green functions (44):

$$\det(\mathbf{E}-\mathbf{H_k})|_{\mathbf{E}=\mathbf{E}_n}\overset{!}{=}0$$

$$E_{1/2}(\mathbf{k})=\frac{1}{2}[2\epsilon(\mathbf{k})-\mathbf{u}\pm\mathbf{\Delta}],$$

$$\Delta=\sqrt{u^2+4t^2}. \tag{52}$$

$\Delta=E_1-E_2$ is a measure for the energetic separation of the layers and depends on the interlayer hopping $t$ set to 0.1 eV and the interlayer-potential difference $u$ induced by the external electric field (23).

Now a simple calculation from Eq. (50) using Eq. (51) yields

$$\overline{p}^{12}(t)=\overline{p}^{21}(t)=4(\alpha^{12})^2\sin^2\left(\frac{t\Delta}{2\hbar}\right), \tag{53}$$

$$\overline{p}^{11}(t)=\overline{p}^{22}(t)=1-\overline{p}^{12}(t), \tag{54}$$

the probability of finding an electron in the second layer ($\overline{p}^{12}$) or in the first layer ($\overline{p}^{11}$) at time $t$ after we prepared it at time $t=0$ in the first layer of our two layer film. Both probabilities are completely determined by $\Delta$, the energetic separation of the layers, and are therefore not $\mathbf{k}$ dependent. Increasing the external electric field $u$, we observe a growing confinement of the electron in the layer it had been prepared in, see Fig. 6. This behavior is well known as Wannier-Stark localization.[25–27]

Finally we want to determine the probability of finding an electron at time $t$ in layer $\beta$ with reversed spin $-\sigma$ after it had been prepared at time $t=0$ in layer $\alpha$ with opposite spin $\sigma$. These spin-flip probabilities $p_{\mathbf{k}\sigma}^{\alpha\beta}(t)$ are obviously given

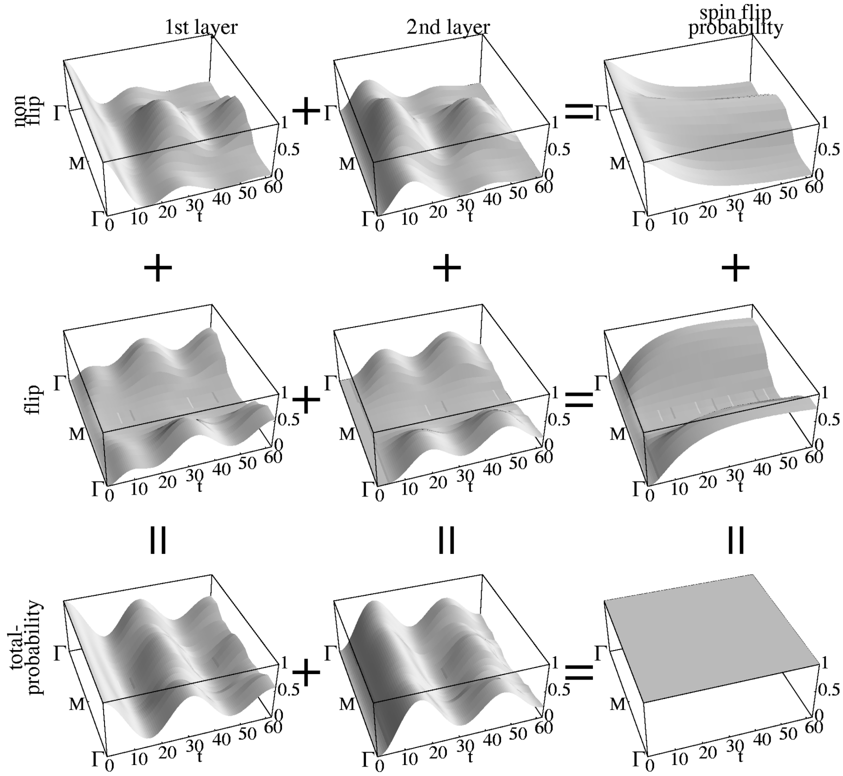


FIG. 7. Spin-flip and nonflip probabilities for a two-layer film with weak $s$-$f$ coupling ($J=0.08$ eV) and without electric field. At $t=0$ a $\sigma=\downarrow$ electron had been prepared in layer one. The first line of pictures shows the time-dependent probability of still being in a $\sigma=\downarrow$ state (in first layer, second layer, somewhere in the system). The second line of pictures shows the probability of being flipped (in first layer, second layer, or somewhere in the system). The bottom line is the sum over both spin directions and gives thus the spin-independent probability of being in the (first layer, second layer, or somewhere in the system). Time is given in $\hbar$/eV$=6.6\times10^{-16}$ sec; the interlayer momentum $\mathbf{k}$ runs from (0,0) to $(2\pi,2\pi)$ through the two-dimensional Brillouin zone.

by the overlap of the Bloch states $|\psi_{\mathbf{k}\alpha\sigma}(0)\rangle=c^{+}_{\mathbf{k}\alpha\sigma}|0\rangle$ with states such as $|\phi^{\beta\gamma}_{\mathbf{kq}-\sigma}(t)\rangle=|S^{\sigma}_{\mathbf{q}\gamma}c_{(\mathbf{k}-\mathbf{q}),\beta,-\sigma}(t)|0\rangle$.

The spin-flip process of the conduction band electron always results from magnon emission, i.e., it is connected to a spin deviation in the lattice of the magnetic $4f$ moments. Let us assume this magnon had been emitted in layer $\gamma$ and carries away the momentum $\mathbf{q}$. In order to get the total spin-flip probability $p^{\alpha\beta}_{\mathbf{k}\sigma}(t)$ we have to sum over all possibilities of emitting such a $(\mathbf{q},\gamma)$ magnon:

$$p^{\alpha\beta}_{\mathbf{k}\sigma}(t)=\sum_{\gamma}\sum_{\mathbf{q}}|\langle\phi^{\beta\gamma}_{\mathbf{kq}-\sigma}(t)|\psi_{\mathbf{k}\alpha\sigma}(0)\rangle|^2. \tag{55}$$

The flip probabilities $p^{\alpha\beta}_{\mathbf{k}\sigma}(t)$ are related to the spectral density $\hat{S}^{\gamma\beta\alpha}_{\mathbf{kq}\sigma}$ of the spin-flip Green function (30) $F^{\gamma\beta\alpha}_{\mathbf{kq}\sigma}=\langle\langle S^{-\sigma}_{-\mathbf{q}\gamma}c_{(\mathbf{k}-\mathbf{q}),\beta,-\sigma};c^{+}_{\mathbf{k}\alpha\sigma}\rangle\rangle$.

A straightforward calculation similar to those in Sec. II B shows

$$p^{\alpha\beta}_{\mathbf{k}\downarrow}(t)=4\pi^2\sum_{\gamma\mathbf{q}}|\hat{S}^{\gamma\beta\alpha}_{\mathbf{kq}\downarrow}(t)|^2. \tag{56}$$

The corresponding probability $p^{\alpha\beta}_{\mathbf{k}\uparrow}(t)$ vanishes, since we considered here the case of a ferromagnetically saturated 4-$f$ lattice, which cannot be aligned any further and thus interdicts spin-flip processes for $(\sigma=\uparrow)$ electrons.

In the last step we have to determine the general spin-flip function $F^{\gamma\beta\alpha}_{\mathbf{kq}\downarrow}$ which is in the usual way connected to its spectral density:

$$\hat{S}^{\gamma\beta\alpha}_{\mathbf{kq}\downarrow}(E)=-\frac{1}{\pi}\,\mathrm{Im}\{F^{\gamma\beta\alpha}_{\mathbf{kq}\downarrow}(E)\}. \tag{57}$$

After Fourier transformation we will get $\hat{S}^{\gamma\beta\alpha}_{\mathbf{kq}\downarrow}(t)$.

The general spin-flip function can be obtained from the hierarchy of the equation of motion. The calculation is comparable to the one in Sec. IV and yields

$$F^{\alpha\gamma\beta}_{\mathbf{kq}\downarrow}(E)=X^{\alpha}(E)G^{\alpha\beta}_{\mathbf{k}\downarrow}(E)G^{\gamma\alpha}_{\mathbf{k}-\mathbf{q}\uparrow}(E), \tag{58}$$

with

$$X^{\alpha}(E)\overset{\mathrm{def}}{=}\frac{J\hbar S}{\sqrt{N_s}}\left(\frac{2}{J\hbar B_{\alpha}(E)-2}\right). \tag{59}$$

Equations (35)–(39) and their generalized form which includes the external electric field (43), (44) completely determine the solution. Equations (56) and (58) give us the probabilities for spin-flip processes we were looking for.

The spin-flip and nonflip probabilities derived so far were evaluated numerically for a two-layer simple cubic film with layers parallel to the (100) face. The results for different values of $s$-$f$ coupling and strengths of the external electric field are shown in Figs. 7, 8, and 9.

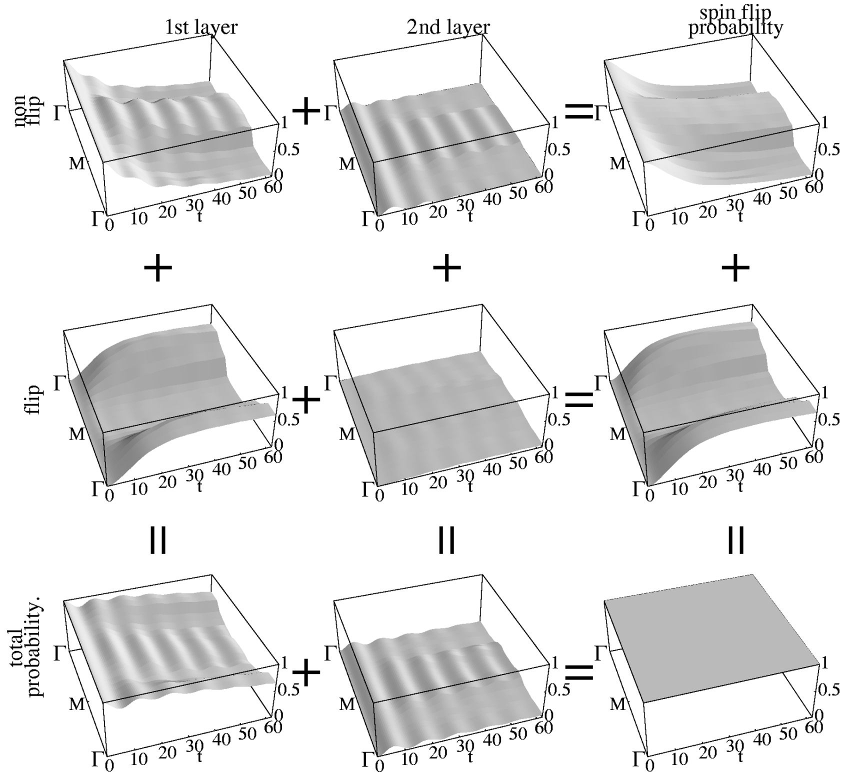


FIG. 8. Same as Fig. 7, but with external electric field ($u=0.4$ eV). The total spin-flip and nonflip probabilities (right column) are, compared to Fig. 7, unchanged, although the individual probabilities changed rather drastically. The spin-totalized probabilities (bottom line) show the Wannier-Stark localization discussed in Sec. (V B): the electron is confined to the layer it had been prepared in.

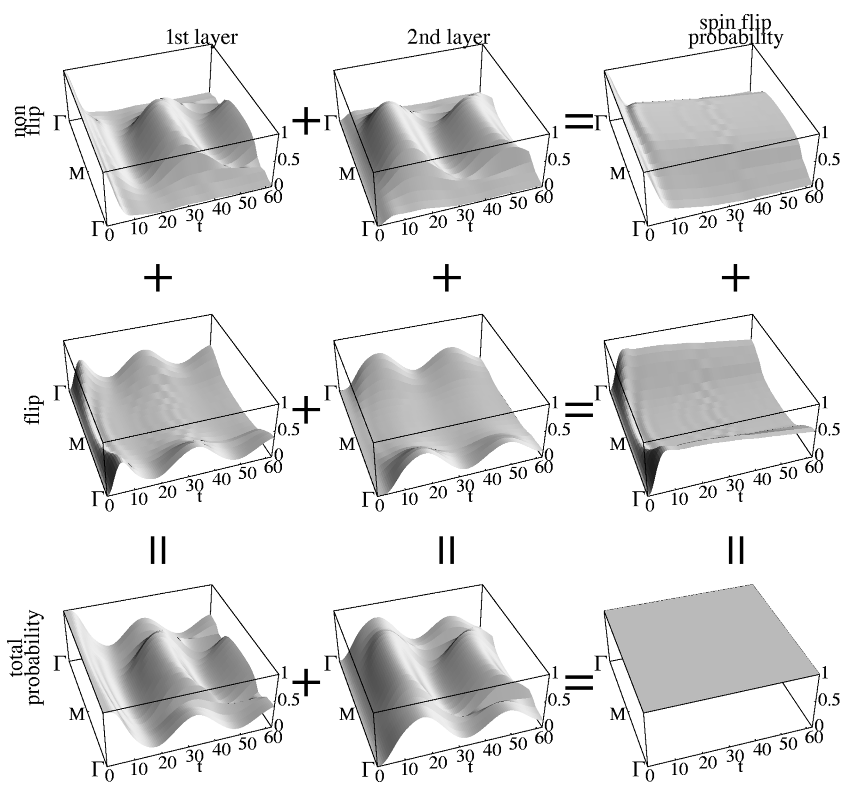


FIG. 9. Same as Fig. 7, but with intermediate $s$-$f$ coupling ($J=0.2$ eV) and without electric field. The total spin-flip and nonflip probabilities (right column) show, compared to Fig. 7, a strong dependence from the $s$-$f$ coupling. The spin-totalized probabilities (bottom line), however, are barely changed.

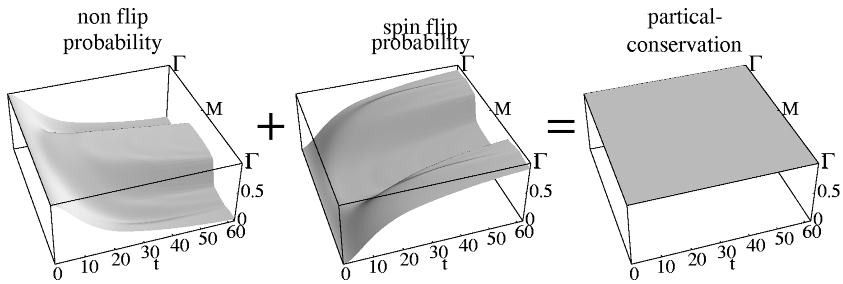


FIG. 10. Nonflip and flip probabilities for a monolayer spin filter with weak $s$-$f$ coupling ($J=0.08$ eV). Time is given in $\hbar/\mathrm{eV}=6.6\times10^{-16}$ sec; the interlayer momentum $\mathbf{k}$ runs from (0,0) to $(2\pi,2\pi)$ through the two-dimensional Brillouin zone. The right picture verifies the particle conservation.

It should be stressed that the shown nonflip and flip probabilities were obtained in separate calculations, based on completely different many-body entities (one-electron Green function and spin-flip function, respectively). However, our understanding of those complementary probabilities demands that they add up to 1 for all times and all vectors $\mathbf{k}$ (particle conservation). As the figures show, this is satisfied in each case (bottom right).

Comparing Figs. 7–10 we can summarize as follows.

(1) The spin-totalized probabilities (bottom lines) do not show a significant dependence on the strength of the $s$-$f$ coupling $J$ between conduction band electrons and localized 4-$f$ moments. Accordingly they are equal to those with no coupling $J\equiv0$ which had been determined analytically in Sec. V B and are completely independent of the intralayer momentum $\mathbf{k}$.

(2) The total spin-flip and nonflip probabilities (right columns) do not show any dependence on the external electric field $u$. Accordingly they are equal to those without field $u\equiv0$.

(3) Calculations for films with various numbers of layers show the total spin-flip and nonflip probabilities are also independent of the total number of layers in the film. Consequently they are the same as those which are calculated for a monolayer.

These observations simplify the practical evaluation of spin-flip probabilities for the spin filter experiment essentially and allow us to determine the polarization of the field-emitted electrons quite generally.

### C. Polarization

According to Eq. (6) the polarization is completely determined by the effective spin-flip ratio $p_{\mathrm{eff}}=p_{\downarrow}-p_{\uparrow}$, where the flip probability for ($\sigma=\uparrow$) electrons $p_{\uparrow}$ vanishes identically and the (time-dependent) flip probability for $\sigma=\downarrow$ electrons $p_{\downarrow}$ is given by Eq. (56) as pointed out in the previous section. Using the observations (2) and (3) concerning $p_{\mathbf{k}\uparrow}^{\alpha\beta}(t)$ made in the previous section the calculation of the polarization simplifies considerably: The dynamics of the spin-flip processes turned out to depend on neither the strength of the external electric field nor the number of layers of the spin filter. It is completely determined by the strength of the $s$-$f$ interaction $J$.

Practically calculating the polarization therefore simply demands that we evaluate the spin-flip probabilities for a monolayer film without electric field $p_{\mathbf{k}\downarrow}$ or, even simpler, its complementary quantity: the nonflip probability $\overline{p_{\mathbf{k}\downarrow}}$ as

$$p_{\mathbf{k}\downarrow}+\overline{p_{\mathbf{k}\downarrow}}\equiv1. \tag{60}$$

In the previous section we showed that after a sufficient long period of time the nonflip probability $\overline{p_{\mathbf{k}\downarrow}}$ is given by the square of the spectral weight of the polaron. This ''critical'' time is characterized by the width of the scattering peak $t\gtrapprox1\hbar/eV=6.6\times10^{-16}$ sec and thus is sufficiently smaller than the typical amount of time an electron spends in the spin filter. We can therefore apply Eq. (49) and obtain finally

$$P_{\mathbf{k}}=p_{\mathbf{k}\downarrow}=1-|\alpha_2(\mathbf{k})|^2. \tag{61}$$

The degree of polarization is completely given in terms of the spectral weight of the magnetic polaron peak $\alpha_2(\mathbf{k})$ and is thus strongly dependent on the $s$-$f$ coupling as well as the electron intralayer momentum $\mathbf{k}$. $\alpha_2(\mathbf{k})$ is obtained by integration of the spectral density (45). Figure 11 shows the degree of polarization $P_{\mathbf{k}}$ calculated according to Eq. (61) for different $s$-$f$ interactions.

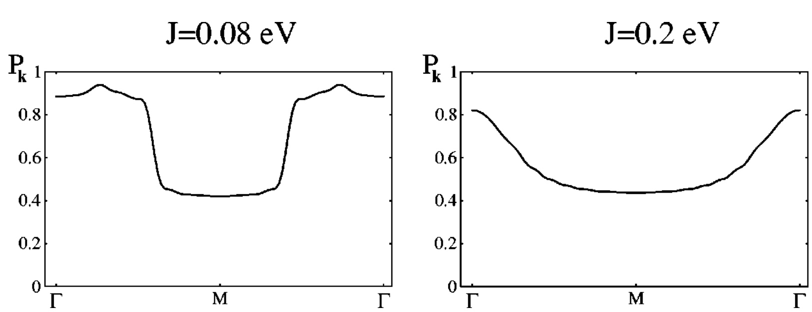


FIG. 11. Degree of polarization $P_{\mathbf{k}}$ according to Eq. (61) for weak ($J=0.08$ eV, left) and intermediate ($J=0.2$ eV, right) $s$-$f$ interactions. The right picture shows the situation for realistic values of $J$ in a spin-filter experiment: $J^{\mathrm{EuS}}\approx0.2$ eV following Wachter (Ref. 1).

It is interesting to see that for unrealistic small values of the coupling ($J \approx 0.08$ eV), one really gets nearly 100% of polarization. This is due to the finite lifetime of the magnetic polarons under these circumstances: The polaronic and scattering peaks touch each other near the origin of the two-dimensional Brillouin zone, the polaronic gets broadened, and the $\sigma = \downarrow$ electrons ''decay'' into ($\sigma = \uparrow$) states. However, for realistic values of $J$ ($J^{\mathrm{EuS}} \approx 0.2$ eV) the polarization lies for all **k** clearly below 100% (Fig. 11, right).

The spin-filter experiment allows only for a **k**-averaged measurement of the degree of polarization $P$. Out of all electrons with given total energy those electrons with maximum energy perpendicular to the tunneling barrier will be transmitted most likely. These are just those electrons with minimum intralayer momentum **k**, i.e., the electrons close to the $\Gamma$ point of the two-dimensional Brillouin zone. According to our calculation (Fig. 11, right) this would yield $P \approx 80\%$, which accounts for the experimental results much better than the former mean field results did.

To exploit Eq. (61) fully, **k**-resolved experiments, such as, for instance, spin polarized low energy electron diffraction or spin polarized electron energy loss spectroscopy on an europium chalcogenide surface are suggested. Because of Eq. (61) one would expect a significant angle, i.e., **k** dependence of the degree of polarization of the scattered electrons (see Fig. 11).

## VI. CONCLUDING REMARKS

The aim of the presented paper was an interpretation of the spin-filter experiments done on europium chalcogenides using recent results from many-body theory on the $s$-$f$ model. This was achieved by expressing the degree of polarization of the field emitted electrons in terms of spin-flip probabilities which had been determined in the framework of an exactly solvable many-body model of the experimental situation. This model used the $s$-$f$ model in reduced dimensions (film geometry), including an additional term taking into account the strong external electrical field. When we discussed the spectral densities of the one-particle Green function, the influence of the external electrical field on electronic behavior was seen, e.g., the Wannier-Stark ladder.

Several physically relevant probabilities such as layer resolved probability densities and flip and nonflip probabilities were derived and discussed, showing, for instance, the Wannier-Stark localization due to the electrical field and the strong dependence of the spin-flip probabilities on the intralayer momentum and the $s$-$f$ coupling between ferromagnetically ordered $4f$ spins and conduction band electrons of the spin filter. The degree of polarization of the field emitted electrons evaluated in our model turned out to be well below 100% for all temperatures which is in good agreement with the experiments and represents considerable progress with respect to the mean field results of former works.

## ACKNOWLEDGMENT

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