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On the exchange-dependent electronic collisions in ferromagnets

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Abstract

This study focuses on the angular and the energy dependence of the exchange scattering between an energetic polarized electron and the conduction band electrons of an itinerant ferromagnet. Upon the collisions the two electrons participating in the scattering process are excited into vacuum levels where their quantum mechanical states, i.e. their wave vectors can be resolved at the same time. The numerical calculations illustrate that the recorded two-particle spectra can be utilized to study the spin-split electronic structure near the Fermi level and to obtain information on the nature of the exchange scattering in ferromagnetic materials.

1. Introduction

The exchange interaction is a vital prerequisite for the occurrence of the long-range magnetic ordering in a variety of materials. This interaction is a result of the fermionic nature of the electrons which implies that the quantum state of a multi-electron system must be antisymmetric with respect to an exchange of any two individual electrons. In the case where the spin degrees of freedom are decoupled from the spatial degrees of freedom one can write the quantum state of an electronic system as a direct product of a spin and a spatial part. If the spin part is antisymmetric with respect to exchange the spatial part must be symmetric and vice versa. Thus, in principle to investigate the exchange interaction one should monitor the scattering of, at least, two electrons with well-defined spin projections and then flip the spin projection of one of the electrons in which case the symmetry of the spin part of the wave function is changed. To obtain a clear picture on the influence of this symmetry operation one should resolve all the relevant quantum numbers of the two electrons before and after the collisions. Experimentally this is a challenging task since the coincident two-electron detection combined with the measurement of the spin-polarization of electrons results in very low-counting rates. Hence, it is only recently that such experiments have been conducted [1–4]. It should be remarked however, that the information obtained by such a coincident technique is restricted to hot electrons, i.e. excited electrons with several eV's above the Fermi level. Electron–electron scattering right at the Fermi level cannot be studied by these methods.

On the theoretical side to describe the state-resolved scattering in an electronic system one has to deal with the excited-state of a many-body system, which is notoriously difficult. In the context of the present work two kinds of correlations have to be treated: (1) Electronic correlation in the

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single-particle ground and excited state of the surface. This situation is akin to other widely used single-particle spectroscopies, such as single photoemission and electron-energy loss spectroscopy. In the calculations shown here electronic correlation of this kind is included on the level of density-functional theory within the local-density approximation. To incorporate the particle-hole spectrum in a more appropriate way we are currently working on utilizing the so-called GW approach [5] for the coincident two-electron spectroscopy. The second kind of correlation that has to be incorporated in the theory is the interaction between the two electrons escaping into the vacuum. This kind of interaction has to be done at least on the two-particle level, since two electrons are detected. The approach of the present study to this part of the problem is first to choose an appropriate model for the electron–electron interaction and then to evaluate numerically the particle–particle propagator. As discussed below the validity of the theoretical model is restricted to the vicinity of the Fermi level E_F. This is reflected by a reasonable agreement between experiment and theory for the spin-dependence of the two-particle spectrum around E_F. However, this agreement turns into a disagreement when the two electrons are emitted from levels considerably lower than E_F. In this case, in contrast to experimental data, the calculations show a strong spin dependence of the emitted two-particle spectrum. The reason for this observation is that the theory does not account for multiple scattering of the emitted electron pairs from other electrons of the conduction band. These processes which are irrelevant at E_F, are strongly spin dependent and are the primely source of the spin decoherence. Thus, in the experiment, only marginal spin dependence is observed away from E_F.

2. Theoretical formulation

2.1. Preliminary remarks

For a concise presentation let us restrict the discussion to the experimental situation studied in [2]. A polarized electron beam with a polarization vector $\boldsymbol{P}_1$ and a wave vector $\boldsymbol{k}_0$ impinges onto a clean ferromagnetic surface (a BCC Fe(1 1 0) in the present study) with a well-defined magnetization direction $\boldsymbol{M}$ (cf. Fig. 1). Upon the interaction of a single electron of the incoming beam with the electronic states in the conduction-band two electrons are emitted with the energies E_1 and E_2 and under certain emission angles θ_1 and θ_2 with respect to the incoming beam direction. The question to be addressed is the following: How does the emission rate of the two electrons change if the direction of $\boldsymbol{P}_1$ or/and $\boldsymbol{M}$ is inverted? In other words the quantity of interest is a spin asymmetry $\mathscr{A}$ which is determined by measuring the electron-pair emission rate W when the magnetization direction (hereafter denoted by $\Downarrow^{\mathrm{M}}$) is antiparallel or parallel to the polarization vector ($\uparrow$) of the incoming beam. The spin asymmetry $\mathscr{A}$ is then evaluated as

$$\mathscr{A}(\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_0)=\frac{W(\uparrow\Downarrow^{\mathrm{M}})-W(\downarrow\Downarrow^{\mathrm{M}})}{W(\uparrow\Downarrow^{\mathrm{M}})+W(\downarrow\Downarrow^{\mathrm{M}})}. \tag{1}$$

For the reaction sketched above the following energy and wave vector balance apply:

$$E_0+\epsilon=E_1+E_2, \tag{2}$$

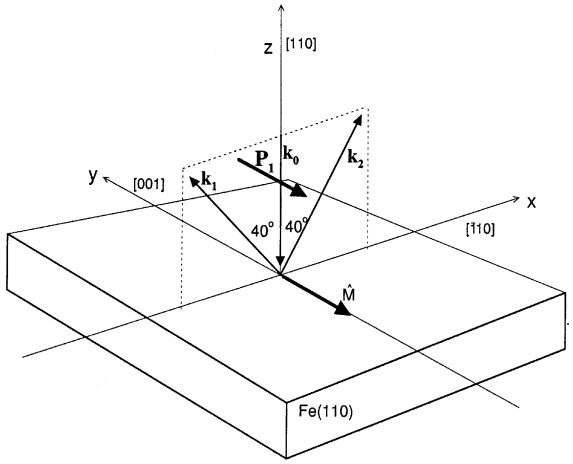

Fig. 1. The experimental set-up as employed for the coincidence measurements shown in Fig. 2. The direction of the magnetization $\boldsymbol{M}$, the spin polarization vector of the incoming beam $\boldsymbol{P}_1$ as well as the wave vectors of the incoming and the two emitted electrons $\boldsymbol{k}_0$, $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ are indicated. The two electrons are detected under an angle of 40° to the left and to the right of the z axis.

$$\boldsymbol{k}_{0\parallel} + \boldsymbol{q}_{\parallel} + \boldsymbol{g}_{\parallel} = \boldsymbol{k}_{1\parallel} + \boldsymbol{k}_{2\parallel}. \tag{3}$$

Here, ϵ is the energy of the valence band electron before it is being excited into the vacuum and $\boldsymbol{q}_{\parallel}$ is its (surface) Bloch wave vector. The surface reciprocal lattice vector is denoted by $\boldsymbol{g}_{\parallel}$. Since we assumed that the quantities E_0, E_1, E_2 and $\boldsymbol{k}_0$, $\boldsymbol{k}_{1\parallel}$, $\boldsymbol{k}_{2\parallel}$ are given by the experiment one can control, via Eqs. (2) and (3), the values of ϵ and $\boldsymbol{q}_{\parallel}$, i.e. one can zoom into certain states in the (magnetic) surface Brillouin zone (BZ). For example we can excite electrons from deeper levels of the conduction band by lowering E_2 while keeping E_1 and E_0 fixed. Equivalently, one can vary $\boldsymbol{q}_{\parallel}$ by changing, e.g., $\boldsymbol{k}_{0\parallel}$ for given $\boldsymbol{k}_{1\parallel}$, $\boldsymbol{k}_{2\parallel}$ and $\boldsymbol{g}_{\parallel}$.

2.2. The two-electron emission probability

The incoming polarized electron beam can be described by the density operator ρ^{s_1} with matrix elements $\rho^{s_1}_{m_{s_1} m_{s_1}}$, where m_{s_1} is the projection of the electron's spin $\boldsymbol{s}_1$. As usual ρ^{s_1} can be expanded linearly in terms of the Pauli matrices σ as

$$\rho^{s_1} = 1 + \boldsymbol{P}_1 \cdot \sigma. \tag{4}$$

To characterize the electrons in the exchange-split conduction band we employ the density matrix $\bar{\rho}^{s_2}_{m_{s_2} m_{s_2}}$, where s_2 is the spin of the electron and m_{s_2} stands for its projection. A representation of the density operator $\bar{\rho}^{s_2}$ is obtained from

$$\bar{\rho}^{s_2} = w_0(\boldsymbol{k}_{2\parallel}, l, \epsilon)(1 + \boldsymbol{P}_2 \cdot \sigma). \tag{5}$$

Here $w_0(\boldsymbol{k}_{2\parallel}, l, \epsilon)$ is the spin-averaged Bloch spectral function of the layer l and $\boldsymbol{P}_2$ is the spin-polarization of the energy and the wave-vector resolved electronic states in the conduction band, i.e.,

$$P_2 = \frac{w(\boldsymbol{k}_{2\parallel}, l, \epsilon, \Uparrow) - w(\boldsymbol{k}_{2\parallel}, l, \epsilon, \Downarrow)}{w_0(\boldsymbol{k}_{2\parallel}, l, \epsilon)}. \tag{6}$$

The quantities $w(\boldsymbol{q}_{\parallel}, l, \epsilon, \Uparrow)$ and $w(\boldsymbol{q}_{\parallel}, l, \epsilon, \Downarrow)$ are the Bloch spectral functions of respectively the majority and the minority bands whereas w_0 is the spin averaged Bloch spectral function. The spectral functions of the sample can be obtained from conventional surface band structure calculations such as the full-potential linearized augmented plane-wave method [8] or from a self-consistent layer-resolved Korringa–Kohn–Rostoker method [9]. These methods are based on the density functional theory within the local-density approximation which works well for the ferromagnetic ground state of iron. The spectral functions are obtained from the trace of the imaginary part of the single-particle Green function g. It has not yet been possible to employ for this kind of studies an expression for g that contains an appropriate self energy function that accounts for the life-time broadening and for the energetic shift the quasi-particle states [5]. In the calculations shown below we assume the imaginary part of the self-energy to be merely a spin-independent constant (0.02 eV).

The cross section W for the simultaneous emission of two electrons with wave vectors $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ in response to the impact of a projectile electron with wave vector $\boldsymbol{k}_0$ is given by

$$W(\boldsymbol{k}_2, \boldsymbol{k}_1, \boldsymbol{k}_0) = C \sum_{m_{s'_1} m_{s'_2}; m_{s_1}, m_{s_2}} \int_{\alpha} \sum T \rho^S T^{\dagger} \delta(E_{\mathrm{f}} - E_{\mathrm{i}}). \tag{7}$$

Here $C = (2\pi)^4/k_0$, $\rho^S = \rho^{s_1} \otimes \bar{\rho}^{s_2}$ and α labels all experimentally non-resolved quantum numbers. In the experiment the spin projections of the final state electrons $m_{s'_1}$, $m_{s'_2}$ are not resolved. This is the reason why we sum over these states in Eq. (7). It should be noted however, that in absence of spin–orbit interaction the total spin S is conserved and there is no need to resolve the total spin state S in the final state once it is known in the initial state.

Eq. (7) involves the matrix elements T of the transition operator $\mathscr{T}$ of the system consisting of the beam electron and the magnetic surface,

$$T(\boldsymbol{k}_1, m_{s'_1}, \boldsymbol{k}_2, m_{s'_2}; \boldsymbol{k}_0, m_{s_1}, \alpha, m_{s_2}) = \langle \psi_{\mathbf{k}_1, \mathbf{k}_2, m_{s'_1}, m_{s'_2}}(1,2) | \mathscr{T} | \phi_{\epsilon, \alpha, s_2, m_{s_2}}(2) \varphi_{\mathbf{k}_0, s_1 m_{s_1}}(1) \rangle. \tag{8}$$

In this relation $\varphi_{k_0, s_1 m_{s_1}}$ is a spinor vacuum state which describes the incoming beam while the single-particle ground state of the surface electron is $\varphi_{k_0, s_2 m_{s_2}}$ (2). The vacuum electron pair is described by the two-particle state vector $|\psi_{\boldsymbol{k}_1, \boldsymbol{k}_2, m_{s'_1}, m_{s'_2}}(1,2)\rangle$.

For the evaluation of (7) the calculation of T has to be carried out. In this work we treat the operator $\mathscr{T}$ to a leading order in the electron–electron and the electron–crystal interaction [7] to arrive at the approximation $\mathscr{T} \approx U_{\rm surf} + U_{\rm ee}(1 + G^{-}_{\rm ee}U_{\rm surf})$. Here $U_{\rm ee}$ is the electron–electron interaction and $G^{-}_{\rm ee}$ is the Green function involving the potential $U_{\rm ee}$. The surface scattering potential is denoted by $U_{\rm surf}$. Spin dependent scattering, such as spin–orbit interactions are neglected in this work. This model takes into account the electron-pair diffraction from the surface crystal potential but it does not account for energy-loss processes of the *electron pair*. According to the energy conservation law (2) these processes are not allowed at the Fermi level, however if electronic levels deeper in the band are involved one has to consider these multiple-step processes. Hence, the above sketched model is justifiable for the electron-pair emission from the vicinity of $E_{\rm F}$ but it is expected to break down if the initially occupied levels are far below $E_{\rm F}$.

In a previous work [6] a group theoretic analysis has been performed to expose the formal structure of the cross section. The portion of the cross section (7) which is of interest for this work has the following structure [6]:

$$W \propto \sum_{\boldsymbol{g}_\parallel, l} w_0(\Lambda_\parallel, l, \epsilon) X_{\rm av}[1 + \mathscr{A}]\delta(E_{\rm f} - E_{\rm i}), \tag{9}$$

where the asymmetry function $\mathscr{A}$ is defined by the relation

$$\begin{aligned}\mathscr{A} &= P_{\rm l}\frac{\sum_l \left[w(\Lambda_\parallel, l, \epsilon, \Downarrow) - w(\Lambda_\parallel, l, \epsilon, \Uparrow)\right]\sum_{\mathbf{g}_\parallel} X_{\rm av} A^s \delta(E_{\rm f} - E_{\rm i})}{\sum_{l'} w_0(\Lambda_\parallel, l', \epsilon)\sum_{\mathbf{g}'_\parallel} X_{\rm av}\delta(E_{\rm f} - E_{\rm i})} \\ &= \frac{W(\uparrow\Downarrow^M) - W(\downarrow\Downarrow^M)}{W(\uparrow\Downarrow^M) + W(\downarrow\Downarrow^M)}.\end{aligned} \tag{10}$$

In these relations we have introduced the wave vectors

$$\Lambda_\parallel = \boldsymbol{K}^{+}_\parallel - \boldsymbol{g}_\parallel - \boldsymbol{k}_{0\parallel}, \quad \boldsymbol{K}^{+}_\parallel = \boldsymbol{k}_{1\parallel} + \boldsymbol{k}_{2\parallel}, \tag{11}$$

and A^s is the "exchange scattering asymmetry" defined as

$$A^s := \frac{X^{(S=0)}(\boldsymbol{k}_1, \boldsymbol{k}_2; \boldsymbol{k}_0, \boldsymbol{g}_\parallel, l) - X^{(S=1)}(\boldsymbol{k}_1, \boldsymbol{k}_2; \boldsymbol{k}_0, \boldsymbol{g}_\parallel, l)}{X^{(S=0)}(\boldsymbol{k}_1, \boldsymbol{k}_2; \boldsymbol{k}_0, \boldsymbol{g}_\parallel, l) + 3X^{(S=1)}(\boldsymbol{k}_1, \boldsymbol{k}_2; \boldsymbol{k}_0, \boldsymbol{g}_\parallel, l)}. \tag{12}$$

As detailed in [2,6], for a given layer, A^s acquires a unity value if the experiment is invariant under an exchange of $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$, for in this situation the triplet scattering is forbidden, i.e. $X^{(S=1)} = 0$. In this highly symmetric case and if we consider a free-standing monolayer or a bulk system the asymmetry (Eq. (10)) takes on the form

$$\mathscr{A} = P_{\rm l}\frac{w(\Lambda_\parallel, \epsilon, \Downarrow) - w(\Lambda_\parallel, \epsilon, \Uparrow)}{w(\Lambda_\parallel, \epsilon, \Downarrow) + w(\Lambda_\parallel, \epsilon, \Uparrow)}. \tag{13}$$

In other words, if an experimental situation is realized for which an exchange of the two emitted electrons has no influence, the spin-polarization of the sample can be imaged by measuring the spin-asymmetry in the two-electron emission spectrum.

3. Numerical results and comparison with experiments

Now we turn to the numerical evaluation of Eq. (10) and to the comparison with experiments. The experiment has been conducted in the geometry shown in Fig. 1. Here we discuss the results for two impact energies $E_0 = 20$ and 27.6 eV. The emission angles θ_1 and θ_2 of the two electrons are measured and have a fixed value of 40°. In the experiment the detectors which are positioned at $\theta_2 = 40°$ and $\theta_1 = 40°$ have however a finite resolution.

The energies of the two electrons are determined and the experiment is performed in a mode where $E_1 = E_2$. This condition ($E_1 = E_2$ and $\theta_1 = \theta_2$), is of a particular interest as it corresponds to the Γ point as deduced from Eq. (3) (in this case $\boldsymbol{k}_{0\parallel} = 0$, $\boldsymbol{k}_{1\parallel} = -\boldsymbol{k}_{2\parallel}$). Therefore, different values of $E_1 = E_2$ correspond to different binding energies $\epsilon = E_1 + E_2 - E_0$ of the conduction band electrons (cf. Eq. (2)) at the Γ point.

In this highly symmetric situation of the set up shown in Fig. 1 ($E_1 = E_2$) the complete experiment and in particular the sample's properties are invariant under a 180° rotation with respect to the $z\|\boldsymbol{k}_0$ direction. On the other hand this symmetry operation is equivalent to an exchange of $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$. Therefore, the triplet scattering vanishes and the term A^s (Eq. (12)) takes on a unity value. This means that the spin asymmetry $\mathscr{A}$ (Eq. (10)) in this case is directly related to the properties of the

electronic band structure of the sample (cf. Eqs. (10) and (13)).

To contrast these statements with experiments it is important to note that the theory has to account for the finite detection solid angles. In the set-up of Fig. 1 the electrons are emitted into a solid angle Ω_θ with an aperture Δ_θ. The sampling over Ω_θ implies an averaging over $\hat{\boldsymbol{k}}_1$ and $\hat{\boldsymbol{k}}_2$ within a certain range. From Eq. (3) it follows that this procedure corresponds to an integration in a certain region in the BZ around the Γ point.

In Fig. 2(a) and (b) we compare the theory with the experiments performed in the set-up shown in Fig. 1 where ϵ is varied by varying E_1 (while keeping the condition $E_2 = E_1$). The angular resolution is $\Delta_\theta = 15°$. As stated above for the strict condition $\theta_1 = \theta_2$ and $E_1 = E_2$ the spin asymmetry $\mathscr{A}$ (Eq. (10)) is an image of the spin-polarization P_2 (cf. Eq. (6)) in the respective region in the BZ. Therefore, the value of $\mathscr{A}$ should not depend on the incident energy E_0 of the beam (since P_2 is independent of E_0). This statement is endorsed by the experimental and the theoretical results for the spin asymmetry near the Fermi level. It should be stressed that the sign and the absolute magnitude of the spin asymmetry is determined by the experiment. The theory performs well near the Fermi level. This is not surprising since the approximation made in the theory are justifiable near E_F. In fact one may perform the experiment such that the energy ϵ is fixed to be near E_F and then scans the asymmetry as function of the crystal momentum $\boldsymbol{q}$, as done in Refs. [2,6]. There it has been also been demonstrated that the theory is capable of describing the behaviour of the spin asymmetry near E_F.

However, if the theory is applied beyond its range of validity, i.e. away from E_F considerable deviations between experiment and theory are observed. This is due to the fact that when the emission occurs from deeper levels in the band the two electrons, before escaping the surface, may scatter from other surrounding electrons losing some of their energies and changing their spin projections (due to the exchange interaction). A sequence of such inelastic energy-loss processes may lead to a complete spin decoherence of the electron pairs and hence to a vanishing spin asymmetry, a behaviour which is indicated by Fig. 2.

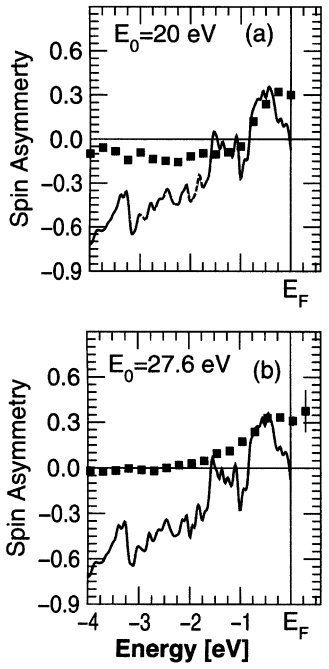

Fig. 2. (a, b) The spin asymmetry $\mathscr{A}$ measured in the set-up shown in Fig. 1. The energies of the two emitted electrons are equal ($E_1 = E_2$). The asymmetry $\mathscr{A}$ is varied as function of the energy $\epsilon = E_1 + E_2 - E_0$. According to Eq. (2) ϵ corresponds to the binding energy of the ground state electrons and hence the Fermi energy is at $\epsilon = 0$. The sets (a) and (b) show the spin asymmetry in the electron-pair spectrum for two different incident energies E_0 of the incoming electrons ($E_0 = 20$ eV in (a) and $E_0 = 27.6$ eV in (b)). In the theory the angular resolution of each of the detectors ($\theta_{1/2} = (40 \pm 15)°$) has been taken into account. Full squares with error bars are experimental data [10] whereas the solid lines are the theoretical results.

This decoherence mechanism is not taken into account by the present theory and hence the disagreement seen in Fig. 2.

Thus it can be concluded, that the present technique is well suited to study the spin polarization of ferromagnets only near the Fermi levels where the energy conservation (Eq. (2)) law forbids inelastic processes of the electron pairs (electrons which lose energy do not escape the surface due to energy considerations).

On the other hand the two-electron coincidence spectroscopy has an advantage in that it is very surface sensitive due to the short escape depth of electrons and since that *two* electrons have to escape the sample. To illustrate this theoretically we

consider in Fig. 3 the spin asymmetry corresponding to the calculations of Fig. 2(a) but the contributions of each of the atomic layers are resolved. As clear from Fig. 3, the positive sign and the magnitude of the spin asymmetry at E_F, as observed in Fig. 2, are basically due to the pair emission from the first layer. The spin asymmetries corresponding to emission from of other layers have negative signs near E_F and their contributions are marginal since the spin asymmetries for the pair emission from the first layer (Fig. 3) resembles well the spin asymmetry in the electron-pair spectrum for emission from the surface (Fig. 2(a)). In contrast, the spin polarization (spin asymmetry) of the third, fourth and fifth layers show already a behaviour very similar to that of a bulk sample and is at variance with the experiments depicted in Fig. 2(a). Here it should be mentioned that the calculations shown in Fig. 2(a) are performed such that the transition matrix elements are calculated for each layer and then these layer and spin-resolved matrix elements are summed coherently. From the coherent sum the cross sections and the spin asymmetries are obtained. That a given layer has a minor contribution means that the transition matrix elements specific to this layer do not deliver appreciable contribution to the coherent sum.

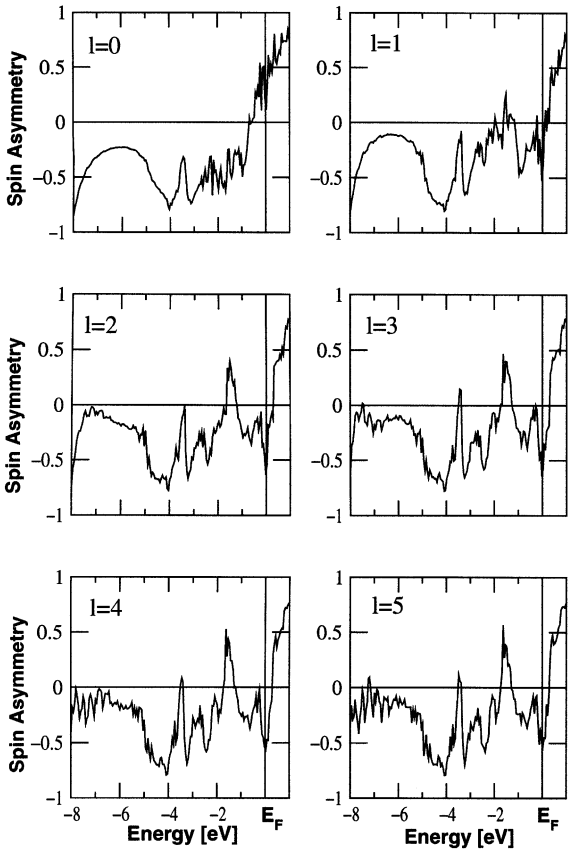

Fig. 3. For the case depicted in Fig. 2(a) we show the spin asymmetry as calculated from the individual atomic layers indexed by l. $l = 0$ is the first atomic layer.

4. Conclusions

This paper deals with the electron-pair emission from magnetic surfaces following the impact of polarized electrons. It has been shown that the electron-pair emission technique can be utilized, under certain conditions, to map out the spin-split electronic band structure of the sample near the Fermi level. Away from E_F spin-dependent inelastic collisions of the electron pair from other electrons lead to a spin decoherence. In addition, a theoretical evidence has been presented for the surface sensitivity of the proposed method.

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