Probing the Spin Polarization in Ferromagnets

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The emission of correlated electrons from an itinerant ferromagnet following the impact of a polarized electron beam is analyzed in terms of irreducible tensorial parameters that can be measured. Under favorable conditions, specified in this work, these parameters are related to the spin polarization in the ferromagnet. The formal results are illustrated by numerical studies of the polarized electron pair emission from a Fe(110) surface, and a novel technique for the investigation of magnetic properties of ferromagnets is suggested.

The electronic and magnetic properties of low dimensional systems with long-range magnetic order, such as ultrathin ferromagnetic films and magnetic surfaces, are currently under intensive investigations [1]. This is due to the fundamental and technological importance of such materials. Magnetic systems with reduced symmetry can be explored by a variety of techniques [1]. Low-energy spin-polarized electron spectroscopy is particularly suitable as the penetration depth is on the order of a few atomic layers [2]. In this method one resolves the quantum states of the incoming and outgoing electrons to extract the accessible information on the sample under investigation. On the other hand, a promising technique emerged in recent years where an electron pair, resolved in energy and momentum, is detected following the impact of an unpolarized electron beam upon a non-magnetic sample [3–6]. As demonstrated successfully for a variety of materials [3–5], the electron pair carries, under favorable conditions, direct signature of the Bloch spectral function which is a central quantity as far as the electronic structure is concerned. However, these studies [3,4] have been performed at higher energies (≈ 20 keV) and the role of the spin polarization has not been yet addressed. Very recently, however, it has been demonstrated by a pioneering experiment [7] that the electron-pair emission depends strongly on the spin polarization of the electron beam and the magnetization of the

sample. Thus, it seems timely to inspect theoretically the low-energy polarized electrons emission from ferromagnets. We conclude the following: (i) the electrons' spectra are quantified fully by a set of irreducible tensorial components; (ii) under certain circumstances specified below, the electron-pair spectrum is directly related to the spin-resolved spectral function of the surface.

For a theoretical formulation we consider a reaction in which two electrons are simultaneously emitted from a ferromagnet with a defined magnetization direction $\hat{\mathbf{M}}$ after the impact of a monoenergetic spin-polarized electron beam. The spins of the electrons in the incoming beam and in the sample are assumed to be good quantum numbers. A corresponding experiment resolves the asymptotic wave vectors of the impinging and the two emitted (vacuum) electrons which we label $\mathbf{k}_1$ and $\mathbf{k}_1'$, $\mathbf{k}_2'$, respectively. No spin analysis of the outgoing electrons is performed. The target surface is described by the state vectors $|\phi_{\epsilon,\alpha,s_2,m_{s_2}}\rangle$, where ϵ is the ground state energy, m_{s_2} is the projection of the spin $\mathbf{s}_2$ of the ground state along a quantization axis, and α denotes all other quantum numbers. The spin polarization of the incoming beam with projection m_{s_1} of the electron's spin $\mathbf{s}_1$ is characterized by the density matrix $\rho_{m_{s_1} m_{s_1}}^{s_1}$, whereas the population of the magnetic sublevels of the state $|\phi_{\epsilon,\alpha,s_2,m_{s_2}}\rangle$ is given by the density matrix $\bar{\rho}_{m_{s_2} m_{s_2}}^{s_2}$. The scattering probability is related to (atomic units, a.u., are used throughout)

$$W(\mathbf{k}_1', \mathbf{k}_2'; \mathbf{k}_1) = C \sum_{m_{s_1'}, m_{s_2'}, m_{s_1}, m_{s_2}} \sum_{\alpha} \mathcal{M}(\mathbf{k}_1', \mathbf{k}_2', m_{s_1'}, m_{s_2'}; \alpha, m_{s_2}, \mathbf{k}_1, m_{s_1}) \rho_{m_{s_1} m_{s_1}}^{s_1} \bar{\rho}_{m_{s_2} m_{s_2}}^{s_2}(\epsilon, \alpha)$$

$$\times \mathcal{M}^*(\mathbf{k}_1', \mathbf{k}_2', m_{s_1'}, m_{s_2'}; \alpha, m_{s_2}, \mathbf{k}_1, m_{s_1}) \delta(E_f - E_i), \qquad (1)$$

where E_f is the final-state total energy. The initial-state total energy E_i is $E_i = E_{\mathbf{k}_1} - \epsilon$, while $E_{\mathbf{k}_1}$ is the energy of the projectile beam and $C = (2\pi)^4/k_1$. All energies are measured with respect to the vacuum level. The transition amplitude $\mathcal{M}(\mathbf{k}_1', \mathbf{k}_2', m_{s_1'}, m_{s_2'}; \alpha, m_{s_2}, \mathbf{k}_1, m_{s_1})$ is given by $\mathcal{M} = \langle \psi_{\mathbf{k}_1', \mathbf{k}_2', m_{s_1'}, m_{s_2'}} | \mathcal{T} | \phi_{\epsilon,\alpha,s_2,m_{s_2}} \varphi_{\mathbf{k}_1, s_1 m_{s_1}} \rangle$, where $\varphi_{\mathbf{k}_1, s_1 m_{s_1}}$ is a spinor vacuum state describing the incoming beam. The emitted electrons with spin projections $m_{s_1'}, m_{s_2'}$ are represented by the state vector $|\psi_{\mathbf{k}_1', \mathbf{k}_2', m_{s_1'}, m_{s_2'}}\rangle$, whereas $\mathcal{T}$ is the transition operator.

In Eq. (1) the density matrices are diagonal. Furthermore, we adopt $\hat{\mathbf{M}}$ as a joint quantization axis for $\mathbf{s}_1$ and $\mathbf{s}_2$. For convenience we express the electrons' final state in the total spin space as $|\psi_{\mathbf{k}_1', \mathbf{k}_2', m_{s_1'}, m_{s_2'}}\rangle = \sum_{SM_S} \langle SM_S | s_1' m_{s_1'}, s_1' m_{s_1'} \rangle |\Psi_{\mathbf{k}_1', \mathbf{k}_2'; SM_S}\rangle$, where S is the total spin and M_S is its projection.

To disentangle geometrical from dynamical properties, we expand the density matrices in state multipoles (statistical tensors) ρ_{pq} [8],

$$\rho^{s_1}_{m_{s_1} m_{s_1}} = \sum_{p_1=0}^{2s_1} (-)^{p_1-s_1-m_{s_1}} \langle s_1 - m_{s_1}; s_1 m_{s_1} \mid p_1 q_1 = 0 \rangle \rho_{p_1 q_1=0}. \tag{2}$$

$$\bar{\rho}^{s_2}_{m_{s_2} m_{s_2}}(\epsilon, \alpha) = \sum_{p_2=0}^{2s_2} (-)^{p_2-s_2-m_{s_2}} \langle s_2 - m_{s_2}; s_2 m_{s_2} \mid p_2 q_2 = 0 \rangle \bar{\rho}_{p_2 q_2=0}(\epsilon, \alpha). \tag{3}$$

Substituting Eqs. (2) and (3) into the general expression (1) yields

$$W = \oint_\alpha \sum_{p_1=0}^{2s_1} \sum_{p_2=0}^{2s_2} \rho_{p_1 q_1=0} \bar{\rho}_{p_2 q_2=0}(\epsilon, \alpha) \Lambda^{p_1,p_2}_{q_1=0,q_2=0} \delta(E_f - E_i), \tag{4}$$

where

$$\Lambda^{p_1,p_2}_{q_1=0,q_2=0} = C \sum_{m_{s_1}} (-)^{p_1-s_1-m_{s_1}} \langle s_1 - m_{s_1}; s_1 m_{s_1} \mid p_1 q_1 = 0 \rangle \sum_{m_{s_2}} (-)^{p_2-s_2-m_{s_2}} \langle s_2 - m_{s_2}; s_2 m_{s_2} \mid p_2 q_2 = 0 \rangle$$

$$\times \sum_{SM_S} \mathcal{M}(\mathbf{k}'_1, \mathbf{k}'_2, SM_s; \alpha, m_{s_2}, \mathbf{k}_1, m_{s_1}) \mathcal{M}^*(\mathbf{k}'_1, \mathbf{k}'_2, SM_s; \alpha, m_{s_2}, \mathbf{k}_1, m_{s_1}). \tag{5}$$

The decisive point is that the sum over m_{s_1} (m_{s_2}) in Eq. (5) defines the component (along $\hat{\mathbf{M}}$) of a spherical tensor of rank p_1 (p_2) [9]. This mathematical observation yields important information as to the transformation behavior of $\Lambda^{p_1,p_2}_{0,0}$: $\Lambda^{p_1=0,p_2}_{0,0}$ ($\Lambda^{p_1,p_2=0}_{0,0}$) is a *scalar* with respect to spin rotations generated by $\mathbf{s}_1$ ($\mathbf{s}_2$), i.e., it represents spin averaged quantities in the $\mathbf{s}_1$ ($\mathbf{s}_2$) spin space, whereas the components $\Lambda^{p_1=\text{odd},p_2}_{0,0}$ ($\Lambda^{p_1,p_2=\text{odd}}_{0,0}$) can be regarded as a spin *orientation* in the $\mathbf{s}_1$ ($\mathbf{s}_2$) spin space (for $p_1 = 1$

it is a polar vector) and, hence, changes sign upon spin reflection, i.e., $\Lambda^{p_1=\text{odd},p_2}_{0,0}(-m_{s_1}) = -\Lambda^{p_1=\text{odd},p_2}_{0,0}(m_{s_1})$ $[\Lambda^{p_1,p_2=\text{odd}}_{0,0}(-m_{s_2}) = -\Lambda^{p_1,p_2=\text{odd}}_{0,0}(m_{s_2})]$. The tensorial components with even p_1 values are alignment parameters, i.e., they describe the deviations in the spectra from the unpolarized case. The above formalism is easily generalized [9] to the case of strong spin-orbit coupling and/or multielectron emission. For two electrons, Eq. (4) reduces to

$$W = \oint_\alpha \left\{ \Lambda^{0,0}_{0,0} \left[\rho_{00}\bar{\rho}_{00} + \rho_{00}\bar{\rho}_{10} \frac{\Lambda^{0,1}_{0,0}}{\Lambda^{0,0}_{0,0}} + \rho_{10}\bar{\rho}_{00} \frac{\Lambda^{1,0}_{0,0}}{\Lambda^{0,0}_{0,0}} + \rho_{10}\bar{\rho}_{10} \frac{\Lambda^{1,1}_{0,0}}{\Lambda^{0,0}_{0,0}} \right] \delta(E_f - E_i) \right\}. \tag{6}$$

The first term of the sum in Eq. (6) is the pair emission rate averaged over the spin orientation of the incoming electron beam and the spin polarization of the sample. The second term describes the spin asymmetry due to the inversion of the magnetization while the incoming electron beam is being *unpolarized*. The third term is the spin asymmetry in the electron-pair emission from *unpolarized targets* when inverting the spin polarization of the electron beam. In the absence of explicit spin interactions in the *transition*

operator $\mathcal{T}$, e.g., spin-orbit coupling, the parameters $\Lambda^{1,0}_{0,0}$ and $\Lambda^{0,1}_{0,0}$ vanish. The last term of Eq. (7) is related to the electron-pair emission from spin-polarized samples by spin-polarized electrons. It is a polar vector both in the $\mathbf{s}_1$ and the $\mathbf{s}_2$ spin spaces, i.e., $\Lambda^{1,1}_{0,0}(-m_{s_1}, m_{s_2}) = -\Lambda^{1,1}_{0,0}(m_{s_1}, m_{s_2}) = \Lambda^{1,1}_{0,0}(m_{s_1}, -m_{s_2})$. The explicit forms of $\Lambda^{1,1}_{0,0}$ and $\Lambda^{0,0}_{0,0}$ are derived from Eq. (5) to be

$$\Lambda^{1,1}_{0,0} = \frac{C}{2} \sum_{S=0}^{1} \sum_{M_s} \{ |\mathcal{M}(\mathbf{k}'_1, \mathbf{k}'_2, SM_s; \mathbf{k}_1, \alpha, \downarrow, \Downarrow)|^2 - |\mathcal{M}(\mathbf{k}'_1, \mathbf{k}'_2, SM_s; \mathbf{k}_1, \alpha, \uparrow, \Downarrow)|^2$$

$$+ |\mathcal{M}(\mathbf{k}'_1, \mathbf{k}'_2, SM_s; \mathbf{k}_1, \alpha, \uparrow, \Uparrow)|^2 - |\mathcal{M}(\mathbf{k}'_1, \mathbf{k}'_2, SM_s; \mathbf{k}_1, \alpha, \downarrow, \Uparrow)|^2 \}, \tag{7}$$

$$\Lambda^{0,0}_{0,0} = \frac{C}{2} \sum_{S=0}^{1} \sum_{M_s} \{ |\mathcal{M}(\mathbf{k}'_1, \mathbf{k}'_2, SM_s; \mathbf{k}_1, \alpha, \downarrow, \Downarrow)|^2 + |\mathcal{M}(\mathbf{k}'_1, \mathbf{k}'_2, SM_s; \mathbf{k}_1, \alpha, \uparrow, \Downarrow)|^2$$

$$+ |\mathcal{M}(\mathbf{k}'_1, \mathbf{k}'_2, SM_s; \mathbf{k}_1, \alpha, \uparrow, \Uparrow)|^2 + |\mathcal{M}(\mathbf{k}'_1, \mathbf{k}'_2, SM_s; \mathbf{k}_1, \alpha, \downarrow, \Uparrow)|^2 \}. \tag{8}$$

The projections of the spins of the sample state and the electron beam parallel (antiparallel) to the quantization axis are labeled, respectively, by the arrows $\Uparrow$ ($\Downarrow$) and $\uparrow$ ($\downarrow$). In the total spin space, Eqs. (7) and (8) are expressed in terms of the singlet and the triplet partial cross sections,

$X^{(S=0)}$ and $X^{(S=1)}$, respectively, i.e.,

$$\Lambda^{1,1}_{0,0} = \frac{C}{2} [X^{(S=1)}(\mathbf{k}'_1, \mathbf{k}'_2; \mathbf{k}_1; \alpha)$$

$$- X^{(S=0)}(\mathbf{k}'_1, \mathbf{k}'_2; \mathbf{k}_1; \alpha)], \tag{9}$$

$$\Lambda_{0,0}^{0,0} = \frac{C}{2} [3X^{(S=1)}(\mathbf{k}_1', \mathbf{k}_2'; \mathbf{k}_1; \alpha)$$
$$+ X^{(S=0)}(\mathbf{k}_1', \mathbf{k}_2'; \mathbf{k}_1; \alpha)] =: 2X^{\text{tot}}. \quad (10)$$

$X^{(S=0)}$ and $X^{(S=1)}$ are determined by the matrix elements, $T^{(S)}(\mathbf{k}_1', \mathbf{k}_2'; \mathbf{k}_1, \alpha)$, of the singlet ($S = 0$) and triplet ($S = 1$) transition operators $\mathcal{T}^S = (\mathbf{1} + (-1)^S \mathcal{P}_{12})\mathcal{T}$. Here, $\mathcal{P}_{12}$ is a permutation operator that interchanges the two emitted electrons. Thus, one obtains the symmetry property $T^{(S)}(\mathbf{k}_1', \mathbf{k}_2'; \mathbf{k}_1; \alpha) = (-1)^S T^{(S)}(\mathbf{k}_2', \mathbf{k}_1'; \mathbf{k}_1; \alpha)$; i.e., in situations where an interchange of the electrons does not modify the ionization dynamics the triplet scattering amplitude and, hence, $X^{(S=1)} = C|T^{(S=1)}|^2$ vanishes. An example will be shown below. Until this point the electronic and structural properties of the sample have not been yet specified. For perfect clean surfaces the integral over α in Eq. (6) implies summation over the surface Bloch wave vector $\mathbf{k}_{2\|}$ and over the surface layers. The Bloch theorem imposes a conservation law for the surface components of the *total* wave vector of the emitted electrons $\mathbf{K}_\|^+ = \mathbf{k}_{1\|}' + \mathbf{k}_{2\|}'$ [10]; i.e., the change of $\mathbf{K}_\|^+$ from its initial value $\mathbf{k}_{1\|} + \mathbf{k}_{2\|}$ (before the collision) is restricted to a multiple of the surface reciprocal lattice vector $\mathbf{g}_\|$. This fact can be used to perform the integrals over $\mathbf{k}_{2\|}$ in Eq. (6) which reduces then to a summation over the surface layers, indexed by l, and over $g_\|$, i.e.,

$$W \propto \sum_{\mathbf{g}_\|, l} \{2X^{\text{tot}}(\mathbf{k}_1', \mathbf{k}_2'; \mathbf{k}_1, \mathbf{g}_\|, l) [\rho_{00}\bar{\rho}_{00}(\epsilon, \Lambda_\|, l)$$
$$+ \rho_{10}\bar{\rho}_{10}(\epsilon, \Lambda_\|, l)A^s(\mathbf{k}_1', \mathbf{k}_2'; \mathbf{k}_1, \mathbf{g}_\|, l)]$$
$$\times \delta(E_f - E_i)\}, \quad (11)$$

where $\Lambda_\| = \mathbf{K}_\|^+ - \mathbf{g}_\| - \mathbf{k}_{1\|}$. The "exchange scattering asymmetry" has been defined as

$$A^s := \frac{X^{(S=1)}(\mathbf{k}_1', \mathbf{k}_2'; \mathbf{k}_1, \mathbf{g}_\|, l) - X^{(S=0)}(\mathbf{k}_1', \mathbf{k}_2'; \mathbf{k}_1, \mathbf{g}_\|, l)}{3X^{(S=1)}(\mathbf{k}_1', \mathbf{k}_2'; \mathbf{k}_1, \mathbf{g}_\|, l) + X^{(S=0)}(\mathbf{k}_1', \mathbf{k}_2'; \mathbf{k}_1, \mathbf{g}_\|, l)}. \quad (12)$$

To calculate the terms in Eq. (11), the state multipoles ρ_{10} and $\bar{\rho}_{10}$ are needed. These can be obtained by inverting the relations (2) and (3). In the standard representation, the density operators of the beam and the surface are linearly expanded in terms of the Pauli matrices $\boldsymbol{\sigma}$ as $\rho^{s_1} = \mathbf{1} + \mathbf{P}_1 \cdot \boldsymbol{\sigma}$ and $\bar{\rho}^{s_2} = w_0(\mathbf{k}_{2\|}, l, \epsilon)(\mathbf{1} + \mathbf{P}_2 \cdot \boldsymbol{\sigma})$, where $w_0(\mathbf{k}_{2\|}, l, \epsilon)$ is the spin-averaged Bloch spectral function of the layer l, and $\mathbf{P}_1$ and $\mathbf{P}_2$ are the polarization vectors. The sample polarization is given by $P_2 =$

$[w(\mathbf{k}_{2\|}, l, \epsilon, \Uparrow) - w(\mathbf{k}_{2\|}, l, \epsilon, \Downarrow)]/[w_0(\mathbf{k}_{2\|}, l, \epsilon)]$. Here $w(\mathbf{k}_{2\|}, l, \epsilon, m_{s_2})$ stands for the spin and layer resolved Bloch spectral function. Thus we obtain $\rho_{00}\bar{\rho}_{00} = [w_0(\mathbf{k}_{2\|}, l, \epsilon)]/2$ and $\rho_{10}\bar{\rho}_{10} = [w_0(\mathbf{k}_{2\|}, l, \epsilon)]P_1 P_2/2$, and Eq. (11) reduces to

$$W \propto \sum_{\mathbf{g}_\|, l} w_0(\Lambda_\|, l, \epsilon)X^{\text{tot}}[1 + \mathcal{A}]\delta(E_f - E_i). \quad (13)$$

The asymmetry function $\mathcal{A}$ has been introduced as

$$\mathcal{A} = P_1 \frac{\sum_l [w(\Lambda_\|, l, \epsilon, \Uparrow) - w(\Lambda_\|, l, \epsilon, \Downarrow)]\sum_{\mathbf{g}_\|} X^{\text{tot}}A^s \delta(E_f - E_i)}{\sum_{l'} w_0(\Lambda_\|, l', \epsilon)\sum_{\mathbf{g}_\|'} X^{\text{tot}}\delta(E_f - E_i)} = \frac{W(\Uparrow\Uparrow) - W(\Downarrow\Uparrow)}{W(\Uparrow\Uparrow) + W(\Downarrow\Uparrow)}. \quad (14)$$

Thus, for the calculation of the tensorial parameters two major ingredients are needed: (i) The spin and layer-resolved spectral function of the sample which can be obtained from the trace of the imaginary part of the corresponding Green function and (ii) the matrix element of the singlet and triplet transition operators. Now we calculate the terms in Eq. (13) for a Fe(110) surface. The Bloch spectral functions used here are provided by two independent calculations: (i) The scalar relativistic full-potential linearized augmented plane-wave method [11,12] and (ii) the full relativistic layer Korringa-Kohn-Rostoker method [2,13]. For the calculations of the transition matrix element we approximate the $\mathcal{T}$ operator by $\mathcal{T} = U_{\text{surf}} + U_{ee}(\mathbf{1} + G_{ee}^- U_{\text{surf}})$, where U_{ee} is the electron-electron interaction, G_{ee}^- is the Green function of the electron pair, and U_{surf} is the surface scattering potential. For U_{surf} we employ, for a given layer, a linear combination of nonoverlapping muffin-tin potentials [10].

As stated above, for certain geometries, the triplet scattering amplitude vanishes due to symmetry and, hence, A^s tends to -1 [cf. Eq. (12)]. Thus, if a monolayer or a bulk system is considered the magnetic asymmetry P_2 can be scanned by determining $W(\Uparrow\Uparrow)$ and $W(\Downarrow\Uparrow)$. This yields a direct (relative) estimate of the population of the spin states in the sample. For multilayered systems, we have to consider the weighting factor X^{tot} in Eq. (14). An example is shown in Fig. 1 for a Fe(110) sample. The two electrons are detected with fixed *equal* energies in the x-z plane and at *symmetric* positions with respect to the z direction while the incident beam direction is varied in the z-y plane. The experiment, in the geometry of Fig. 1, is invariant under a 180° rotation with respect to the z direction. This rotation can be regarded as an interchange of $\mathbf{k}_1'$ by $\mathbf{k}_2'$ and, since $T^{(S=1)}(\mathbf{k}_1', \mathbf{k}_2'; \mathbf{k}_1, \alpha) = -T^{(S=1)}(\mathbf{k}_2', \mathbf{k}_1'; \mathbf{k}_1, \alpha)$, the triplet scattering ($X^{(S=1)} = C|T^{(S=1)}|^2$) vanishes.

The energies ϵ in Eq. (14) are determined by $\epsilon = E_1' + E_2' - E_{\mathbf{k}_1}$, where E_1' and E_2' are the energies of the vacuum electrons. Thus we tune E_1', E_2', and $E_{\mathbf{k}_1}$ such that ϵ coincides with the Fermi energy E_F. Now by varying $\beta = \cos^{-1}\hat{\mathbf{z}} \cdot \hat{\mathbf{k}}_1$ we scan P_2 along
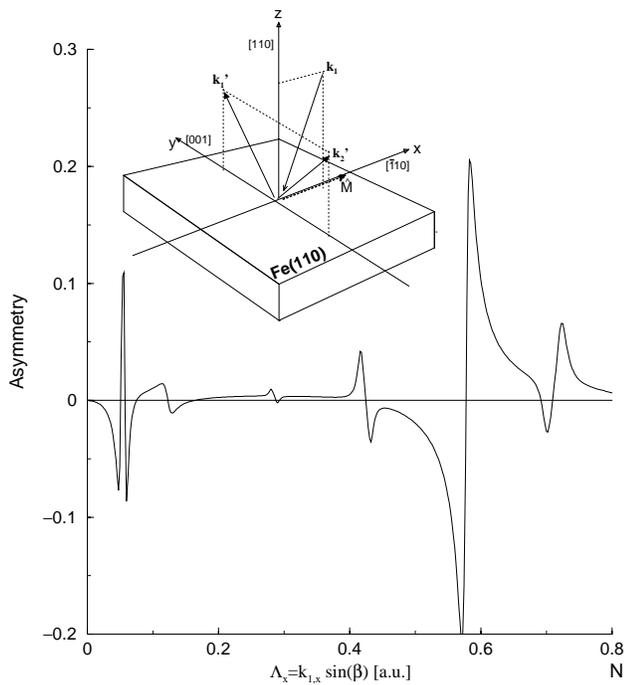
FIG. 1.   The asymmetry, as given by Eq. (14), for the emission of two equal-energy electrons from a magnetized Fe(110) surface following the impact of a polarized electron beam with an energy of 35 eV.   The total energy of the pair is fixed to $E'_1 + E'_2 = 30.15$ eV.   The two electrons are detected in the y-z plane at symmetric position $\cos^{-1}\hat{\mathbf{z}} \cdot \hat{\mathbf{k}}'_1 = 40° = \cos^{-1}\hat{\mathbf{z}} \cdot \hat{\mathbf{k}}'_1$ left and right to the z axis (cf. inset) and $\hat{\mathbf{M}} \parallel x$.   The angle of incidence $\beta = \cos^{-1}\hat{\mathbf{z}} \cdot \hat{\mathbf{k}}_1$ is varied in the x-z plane, as shown by the inset.   In this geometry, the triplet scattering vanishes and $\mathcal{A}$ can be related to P_2.   The predominant contributions to $\mathcal{A}$ originate from the first and second surface layers.

FIG. 2.   The spin asymmetry $\mathcal{A}$ as a function of the energy sharing $(E'_1 - E'_2)/(E'_1 + E'_2)$ for a fixed total energy $(E'_1 + E'_2) = 21$ eV.   The incident electron has an energy 26 eV and a polarization degree of $\approx 65\%$.   This is the same target as in Fig. 1, however, we choose $\beta = 0$ and the two electron detectors to lay in the x-z plane.   As in Fig. 1, the detectors are positioned at $\cos^{-1}\hat{\mathbf{z}} \cdot \hat{\mathbf{k}}'_1 = 40° = \cos^{-1}\hat{\mathbf{z}} \cdot \hat{\mathbf{k}}'_1$.   The theoretical results are averaged over the angular resolution of the detectors.   The experimental data are courtesy of Ref. 7.   The spectral functions are calculated within the scalar relativistic full-potential linearized augmented plane-wave method [11].

the Γ-N direction in the Brillouin zone, as shown in Fig. 1. Alternatively, one may fix the direction $\Lambda_\parallel = \mathbf{k}_{1\parallel}$ and image $P_2(\epsilon)$ by varying, e.g., the incident energy. For a polarized homogeneous electron gas, one scans (as function of energy) the relative difference between the occupied density of states of the majority and minority bands.

Away from the points of high symmetry (cf. Fig. 1) the scattering dynamics, as described by $X^{(S=0)}$ and $X^{(S=1)}$ become dominant. An example is shown in Fig. 2 for $\beta = 0$. Again at the Γ point ($\mathbf{k}'_{1\parallel} = -\mathbf{k}'_{2\parallel}$) the asymmetry $\mathcal{A}$, and in particular its sign, is determined solely by P_2. The For highly asymmetric energy sharing the scattering exchange asymmetry A^s is small which leads to a reduced asymmetry $\mathcal{A}$, as seen in Fig. 2.

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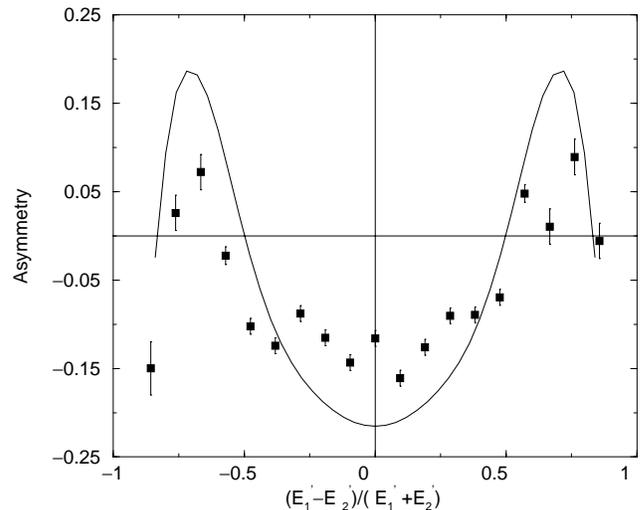
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