Spin polarization and relativistic electronic structure of the $1 \times 1$ H/W(110) surface

Asier Eiguren$^{1,3}$ and Claudia Ambrosch-Draxl$^2$

$^1$ Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, 20018 Donostia/San Sebastian, Spain
$^2$ Department of Materials Physics, University of Leoben, Franz-Josef-Straße 18, A-8700 Leoben, Austria
E-mail: asier.eiguren@ehu.es

New Journal of Physics 11 (2009) 013056 (12pp)
Received 19 September 2008
Published 30 January 2009
Online at http://www.njp.org/
doi:10.1088/1367-2630/11/1/013056

Abstract. We present an analysis of the relativistic electronic structure of the $1 \times 1$ H/W(110) surface. Our calculations reproduce in detail the experimentally determined Fermi surface and spin polarization of the surface electron states. A projected spin-polarized density of states is defined in order to simulate the photoemission spectra exhibiting very good agreement with existing spin-resolved measurements. Our calculations confirm that the spin-split states, $S_1$ and $S_2$, are approximately circularly spin polarized with respect to the high-symmetry point $\bar{S}$. Moreover, we present the precise shape and magnitude of the spin polarization of the spin–orbit split $S_1$ and $S_2$ states, through the entire Brillouin zone.

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$^3$ Author to whom any correspondence should be addressed.
1. Introduction

Since the rather unexpected discovery of spin polarization (and spin splitting) of the Shockley-type surface state in the Au(111) surface [1], this phenomenon has attracted considerable interest due to its relevance in the emergent field of spintronics [2]. An enormous effort is being concentrated in order to produce and understand device functions based on the electron spin. The spin polarization phenomena in nominally non-magnetic surfaces have been intensively studied, and it is established that their origin resides in the lack of inversion symmetry in the surface area, as originally proposed by LaShell et al [1]. Among the several surfaces and interface systems where the spin polarization accompanied by spin splitting has been observed, we mention the bare surfaces W(110) [3, 4], Bi(110) [5], Bi(111) [6] and Cr(110) [7, 8], as well as the quasi-one-dimensional Au/Si(557) system [9] and the more recently studied thin film systems of Au and Ag [10].

The 1 × 1 hydrogen covered tungsten (110) surface (1 × 1 H/W(110)) is another prominent example where surface states provide evidence for a spin-split Fermi surface [4]. In the last two decades, this system gained special relevance because of the anomalies in the W(110) substrate-derived phonon modes [11]–[13], and the measured strong coupling between the surface electrons and the hydrogen-derived phonon branches [14]–[16]. In this paper, we focus on describing the relativistic electronic structure of the 1 × 1 H/W(110) surface considering the non-collinear spin formalism within density functional theory (DFT) [17, 18]. As will be shown, the utilization of a non-collinear approach turns out crucial for understanding the momentum dependence of the spin polarization of the surface states.

2. Theoretical approach

We start by very briefly introducing the formalism to treat spin–orbit (SO) coupling and non-collinear magnetism within DFT. In standard Hohenberg–Kohn–Sham theory, i.e. disregarding spin, an effective one-particle Schrödinger equation, the Kohn–Sham (KS) equation, has to be solved self-consistently. Thereby the electron density is built up by contributions from a set of auxiliary non-interacting single-particle wavefunctions, the KS orbitals. The extension of the Hohenberg–Kohn theorem [19] to the spin-polarized case is not straightforward, since there is no unique one-to-one correspondence between the spin-dependent potential and the spin-dependent density. However, as derived by von Barth and Hedin [17], a generalization of the KS scheme leads (in the simplest approximation) to the solution of two coupled equations for the components of the spinor wavefunctions. Thereby the external scalar potential has to be replaced by a spin-dependent one, \( V_{\text{ext}}^{\sigma\sigma'} \), and the electron density, \( \rho(\mathbf{r}) \), by the density matrix

\[
n_{\sigma'^{\sigma}}(\mathbf{r}) = \sum_{k,n} \psi_{k,n}^{\sigma'}(\mathbf{r})^\ast \psi_{k,n}^{\sigma}(\mathbf{r}) = \frac{1}{2} (\rho(\mathbf{r}) \mathbb{I} + \mathbf{\sigma} \cdot \mathbf{m}(\mathbf{r})) ,
\]

\[
n_{\sigma'^{\sigma}}(\mathbf{r}) = \frac{1}{2} \begin{pmatrix} \rho(\mathbf{r}) + m_z(\mathbf{r}) & m_x(\mathbf{r}) - im_y(\mathbf{r}) \\ m_x(\mathbf{r}) + im_y(\mathbf{r}) & \rho(\mathbf{r}) - m_z(\mathbf{r}) \end{pmatrix} ,
\]

which depends on the ordinary electron density

\[
\rho(\mathbf{r}) = \sum_{k,n,\sigma} \psi_{k,n}^{\sigma}(\mathbf{r})^\ast \psi_{k,n}^{\sigma}(\mathbf{r})
\]
as well as on the magnetization density

\[ m(r) = \sum_{k,n,\sigma,\sigma'} \psi_{k,n}^{\sigma'}(r)^\dagger \sigma_{\sigma,\sigma}^{\sigma'} \psi_{k,n}^{\sigma}(r) \equiv \sum_{k,n} \sigma_{k,n}(r). \]  

(4)

The generalized KS equations take the form of a Pauli equation formulated in terms of two-component spinor wavefunctions,

\[ \sum_{\sigma'} \left[ \left( -\frac{1}{2} \nabla_r^2 + v_H(r) \right) \delta_{\sigma\sigma'} + V_{\text{ext}}^{\sigma\sigma'}(r) + V_{xc}^{\sigma\sigma'}(r) \right] \psi_{k,n}^{\sigma'}(r) = \epsilon_{k,n} \psi_{k,n}^{\sigma}(r), \]  

(5)

where the Hartree potential \( v_H(r) \) together with the kinetic energy represent the spin-diagonal contributions to the Hamiltonian. The external potential \( V_{\text{ext}}^{\sigma\sigma'}(r) \) as well as the exchange–correlation (xc) potential, \( V_{xc}^{\sigma\sigma'}(r) \equiv \delta E_{xc}/\delta n_{\sigma\sigma}(r) \), are generally described by non-diagonal 2×2 matrices and couple the angular and spin degrees of freedom.

For collinear systems, the off-diagonal components of the generalized density vanish, and the KS system can be solved by two independent equations for the spin-up and spin-down states. The exchange correlation potential is obtained by the functional derivative of the exchange correlation energy with respect to the charge density associated with each spin and the local spin-density approximation (LSDA) is commonly used for the xc terms. In the non-collinear case, the equivalent to the LSDA works by finding a local reference frame where the density matrix appears diagonal, such that the collinear spin functionals are applicable locally, i.e. in each point in space \([18]\). The generalized gradient approximation (GGA) can also be introduced in the formalism \([20]\). Non-collinearity appears through the non-diagonal elements of the total effective potential matrix, \( V_{\text{eff}}^{\sigma\sigma'}(r) = V_{\text{ext}}^{\sigma\sigma'}(r) + V_{xc}^{\sigma\sigma'}(r) \), which is the origin of the unrestricted orientation of the effective magnetic field acting on the electron spin. Using matrix notation, it is easy to find that (in matrix notation)

\[ V_{\text{eff}}(r) = \frac{1}{2} (v_{\text{eff}}(r) I + \sigma \cdot B_{\text{eff}}(r)), \]  

(6)

where, in terms of the four components of the potential, \( V_{\text{eff}}^{\sigma\sigma'} \), the scalar potential and the effective magnetic field are written as

\[ v_{\text{eff}} = V_{\text{eff}}^{\uparrow\uparrow} + V_{\text{eff}}^{\downarrow\downarrow} \]  

(7)

and

\[ B_{\text{eff}} = \begin{pmatrix} B_x \\ B_y \\ B_z \end{pmatrix} \equiv \begin{pmatrix} V_{\text{eff}}^{\uparrow\uparrow} + V_{\text{eff}}^{\downarrow\downarrow} \\ i(V_{\text{eff}}^{\uparrow\downarrow} - V_{\text{eff}}^{\downarrow\uparrow}) \\ V_{\text{eff}}^{\downarrow\downarrow} - V_{\text{eff}}^{\uparrow\uparrow} \end{pmatrix}, \]  

(8)

respectively.

The electron spin itself has a relativistic origin, but we have not explicitly mentioned relativity so far. The SO interaction is one of the most important relativistic corrections together with the Darwin and the mass–velocity factors, where the former can be straight-forwardly included in the scalar potential (scalar-relativistic effects). The classical picture of the SO interaction corresponds to the coupling between the electron spin and the self-induced magnetic field due to the orbital motion. In contrast to the scalar-relativistic effects, SO coupling needs, in general, the spinor form of the wavefunctions. In principle, a fully relativistic treatment of DFT requires the substitution of the effective Schrödinger equation by the Dirac equation \([21]–[23]\).
However, including the SO term as an additional correction to the scalar relativistic calculations has been proved to be very satisfactory for most purposes in solid state physics.

A standard procedure to treat relativity within the pseudopotential formalism is to consider the non-relativistic KS–Pauli scheme (equation (5)) together with pseudopotentials generated by considering the full Dirac equation. As shown by Kleinman [24], this approach introduces relativistic corrections up to $\alpha^2$ (with $\alpha$ being the fine-structure constant), representing an enormous simplification over the self-consistent solution of the Dirac equation. In this way, the pseudopotential plays the role of the $2 \times 2$ external potential in equation (5) and carries the essential information about the SO interaction. Within this procedure one basically forces the spinor wavefunctions to match the Dirac solutions in the atomic region (as a kind of boundary condition) and the relativistic effects in the interstitial area are mostly neglected. This turns out to be a very good approximation, particularly for valence electrons [24, 25].

The relativistic electronic structure has been obtained by the non-collinear version of the LSDA approach and including the SO interaction utilizing the PWSCF code [25, 26].

3. Results

To investigate the surface system, we apply the repeated slab approach. The unit cell consists of 15 W(110) layers plus two additional hydrogen layers, one at each side of the slab, representing a full monolayer coverage of the surface. The system was considered relaxed when the forces acting on each of the atoms were smaller than $10^{-5}$ Ryd au$^{-1}$. The so obtained structure agrees with earlier scalar-relativistic calculations [13, 16, 27].

Figure 1 shows the calculated Fermi surface of the slab system. The grey area represents the bulk-projected electron bands, and the orange and black solid lines indicate the scalar relativistic and the relativistic calculations, respectively. The projected bulk electron bands were obtained from a relativistic calculation of the bulk tungsten using a very dense momentum sampling. The reason why the grey area does not appear completely filled by the Fermi contours lies in the fact that the slab system is finite, i.e. taking into account 15 tungsten layers only. However, the band energies and both the Fermi surfaces are almost completely doubly degenerate, demonstrating that the considered number of layers is sufficient for simulating the surface system. Moreover, even 7 W layers turned out to reproduce the surface electron band structure [16]. Within the bulk area, the scalar relativistic and the relativistic results almost coincide, indicating—as expected—that the SO splitting is almost a pure surface phenomenon.

Experimentally, the electronic structure of this system was studied by angular-resolved photoemission spectroscopy (ARPES) [4]. Thereby the authors concentrated on the high-symmetry direction $\vec{\Gamma}--\vec{\Delta}$, reporting the degree of spin polarization as well as the band energies of the two spin-split surface electron states, labelled $S_1$ and $S_2$. The calculated Fermi surface sheets arising from $S_1$ and $S_2$ are indicated in figure 1 and show almost perfect agreement with the experimentally determined Fermi contours [4]. The orange line located approximately in the middle between $S_1$ and $S_2$ shows the spin-degenerate $S$ state (in the absence of SO interaction). Concerning the wave vectors $\mathbf{k}_1$ and $\mathbf{k}_2$ marked in the figure, we will come back below with an analysis of the spectral line shapes reported in [4]. Figure 1 also allows to estimate to what extent the surface states are (de)localized, when they penetrate more deeply into the bulk region as the electron band approaches the surface-projected bulk band area.

Figure 2 shows the calculated relativistic band structure. Like in figure 3 the grey area comes from the bulk-projected electron bands, whereas solid black lines indicate the surface bands of this system, where the only ones crossing the Fermi level are $S_1$ and $S_2$. Figure 3
Figure 1. Fermi surface of the $1 \times 1$ H/W(110) surface system. The grey area indicates the bulk-projected bands; solid orange and black lines represent the relativistic and scalar-relativistic results, respectively. The surface states $S_1$ and $S_2$ around the high-symmetry point $\bar{S}$ originate due to spin splitting in the presence of the SO interaction.

Figure 2. Band structure of the $1 \times 1$ H/W(110) surface along high-symmetry directions. Solid (black) lines are the relativistic electron bands, whereas the grey area originates from the bulk-projected bands. The two spin-split surface states, $S_1$ and $S_2$, are especially visible along $\bar{\Gamma} - \bar{S}$ and $\bar{H} - \bar{P}$. The dashed–dotted (red) vertical lines indicate the wave vectors for which further analysis is provided in figures 4 and 5.
Figure 3. Electron band structure along $\Gamma - \bar{S}$ and $\bar{H} - \bar{P}$ representing a zoom into figure 2.

allows for a better resolution of the electronic structure by zooming into the region around $E_F$ along the high-symmetry directions $\bar{S} - \Gamma$ and $\bar{H} - \bar{P}$. The measured band structure along $\bar{S} - \Gamma$ (figure 1 of [4]) agrees very well with our calculations in terms of dispersion and spin splitting. The calculated Fermi crossing points along the $\bar{S} - \Gamma$ direction are $k_F(S_2) \sim 0.56 \text{ Å}^{-1}$ and $k_F(S_1) \sim 0.70 \text{ Å}^{-1}$ for $S_2$ and $S_1$, respectively, comparing well with the experimentally determined values [14] of $k_F(S_2) \sim 0.46 \text{ Å}^{-1}$ and $k_F(S_1) \sim 0.65 \text{ Å}^{-1}$. Close to the $\bar{\Gamma}$ point, where the bottom of the surface bands is located, the $S_1$ and $S_2$ states become resonance states, overlapping with the bulk-projected bands. The measured minimum of $S_1$ is found at approximately $E_S(S_1(\Gamma)) \sim -1.45 \text{ eV}$ (figure 1 of [4]), whereas it is $E_S(S_2(\Gamma)) \sim -0.85 \text{ eV}$ for $S_2$. We find $E_S(S_1(\Gamma)) = -1.50 \text{ eV}$ and $E_S(S_2(\Gamma)) = -1.01 \text{ eV}$. Our calculations also reproduce the high bulk density of states (DOS) located at around $-1.75 \text{ eV}$ in experiment [4]. The overall agreement is very good but these results suggest that the experimentally determined Fermi energy could be shifted by $\sim 0.1 \text{ eV}$ with respect to our calculations. This is consistent with the values that we would obtain for the calculated Fermi crossing points by shifting the Fermi energy downward by this amount. In this way, we would obtain $k_F(S_2) \sim 0.51 \text{ Å}^{-1}$ and $k_F(S_1) \sim 0.66 \text{ Å}^{-1}$, which would result in an even closer agreement with photoemission measurements. Studying the effects of slab thickness and xc functional (by using GGA rather than local density approximation (LDA)) we find that the band energies do not significantly change. Hence, we conclude that the possible slight offset between theory and experiment must either be attributed to the deviation of the quasiparticle band from the KS band structure or to the experimental determination of the Fermi edge.

In practical implementations of the ARPES, the quantized spin states cannot be measured in the same way as in the Stern–Gerlach (SG) experiment. This is due to the net charge of electrons (in contrast to neutral atoms in the SG experiment) that are strongly deflected in a finite magnetic field [28, 29]. After a preselected electron beam is obtained with certain energy...
and momentum (as in regular ARPES), the information about the spin polarization is obtained by passing the beam through an additional spin-dependent scatterer [28]. This procedure gives rise to a spin-resolved photoemission intensity, $D_u^+(\mathbf{k}, \omega)$, for a given spin quantization direction, $\mathbf{u}$, defined by the scattering geometry.

We estimate the spin-resolved ARPES spectra by adopting the simplest possible picture, where all inherent many-body effects are neglected and the photoemission matrix elements are considered independent of the electron state, i.e. taken to be constant. Within these approximations, the spin-integrated ARPES spectra are expected to be proportional to the electron DOS for a given wave vector $\mathbf{k}$

$$D(\mathbf{k}, \omega) = \sum_{n,\sigma,\sigma'} \delta(\omega - \epsilon_{n,k}) \int \psi_{n,k}^{\sigma'}(\mathbf{r})^\ast \delta_{\sigma',\sigma} \psi_{n,k}^\sigma(\mathbf{r}) \, d^3r, \quad \text{(9)}$$

where $\{\delta_{\sigma',\sigma}\} \equiv \mathbb{I}$ denotes the identity matrix.

Let $\sigma_{k,n}(\mathbf{r})$ be the expectation value of the spin for a particular electron state with wave vector $\mathbf{k}$ and band index $n$ (see equation (4)). We simulate the spin-resolved photoemission intensity by the total probability of finding an electron with the same direction and polarization as defined by the vector $\mathbf{u}$ (determined by the analyser geometry)

$$D_u^+(\mathbf{k}, \omega) = \sum_n \delta(\omega - \epsilon_{n,k}) \int (\sigma_{k,n}(\mathbf{r}) \cdot \mathbf{u}) \, \theta (\sigma_{k,n}(\mathbf{r}) \cdot \mathbf{u}) \, d^3r \quad \text{(10)}$$

and $\theta$ representing the Heaviside function. The spectrum for the opposite direction, $-\mathbf{u}$, is

$$D_u^-(\mathbf{k}, \omega) = \sum_n \delta(\omega - \epsilon_{n,k}) \int (-\sigma_{k,n}(\mathbf{r}) \cdot \mathbf{u}) \, \theta (-\sigma_{k,n}(\mathbf{r}) \cdot \mathbf{u}) \, d^3r. \quad \text{(11)}$$

The spin-integrated spectra are given by the sum of the positive definite functions $D_u^+(\mathbf{k}, \omega)$ and $D_u^-(\mathbf{k}, \omega)$, as $D_u = D_u^+ + D_u^-$, and the degree of spin polarization can be defined as

$$P_u(\mathbf{k}, \omega) = \frac{D_u^+(\mathbf{k}, \omega) - D_u^-(\mathbf{k}, \omega)}{D_u^+(\mathbf{k}, \omega) + D_u^-(\mathbf{k}, \omega)}. \quad \text{(12)}$$

Due to computational reasons, it is convenient to construct a slab system, which is symmetric under inversion. However, as mentioned in the introduction, the absence of inversion symmetry is responsible for the spin splitting when SO interaction is present. In any case, the above picture is not contradicted by the symmetric slab, because the additional degeneracy introduced by both equivalent surfaces allows for two separate surface states, differing only by parity, each of them with opposite magnetization close to each surface (compensated for the overall slab). In this way, each surface separately, behaves effectively as if only time reversal were present, and all the expectation values, such as in equations (10) and (11), are calculated considering only one-half of the slab system.

The wave vectors $\mathbf{k}_1$ and $\mathbf{k}_2$ indicated in figures 2 and 3 are close to the ones for which in [4] the spin-polarized ARPES spectra are presented. In these two points we simulate such spectra as given by equations (10)–(12). Panels (a) of figures 4 and 5 show the degree of spin polarization, $P_u(\mathbf{k}, \omega)$, at $\mathbf{k}_1$ and $\mathbf{k}_2$, respectively. In panels (b)–(d) the spin-resolved DOS, $D_u^+$ (solid) and $D_u^-$ (dashed), are shown for several directions. They correspond to the cases where $\mathbf{u}$ is parallel ($\mathbf{k}_1$, panel (b)), perpendicular to the electron momentum ($\mathbf{k}_\perp$, panel (c)), and perpendicular to the surface ($\hat{z}$, panel (d)).
Figure 4. Spin analysis for the wave vector \( k_1 \) indicated in figures 1 and 2. (a) Solid (black) and dotted (red) lines represent the electron polarization (equation (12)) parallel (\( u = k_\parallel \)) and perpendicular (\( u = k_\perp \)) to the electron wave vector, respectively. The dashed line shows the very small polarization perpendicular to the surface. (b) Spin-projected DOS parallel to the electron momentum, i.e., \( u = \hat{k}_\parallel \) in \( D^\pm_{k_\parallel}(E) \) and \( D^\pm_{k_\perp}(E) \) (arbitrary units) in equations (10) and (11), (c) same for \( u = \hat{k}_\perp \), and (d) \( u = \hat{z} \).

In [4] the measured counterparts of \( D^\pm_u(k, \omega) \) are presented for \( u \) parallel to the photoelectron momentum in the \( \bar{\Gamma} - \bar{S} \) direction, perpendicular to \( \bar{\Gamma} - \bar{S} \) (almost tangential to the Fermi surface of \( S_1 \)), as well as for \( u \) perpendicular to the surface normal. Thus, panel (c) can be directly compared with experiment. The agreement is excellent, showing that the spin structure obtained between \(-1.5 \text{ eV} \) and the Fermi level is described correctly for both surface states. Specifically, the lower energy peak around \(-1.0 \text{ eV} \) in figure 4 corresponds to \( S_1 \), whereas the one at \(-0.3 \text{ eV} \) originates from \( S_2 \). At these two energies, we find almost 100% polarization in either direction in close agreement with experimental results. The almost negligible spin polarization in the energy ranges around \(-4 \) and \(-1.5 \text{ eV} \), as well as the shape of the spectra are very well described by our calculations. The dotted (red) line in panel (a) demonstrates that the polarization parallel to the electron wave vector is not negligible, but reaches values...
Figure 5. Spin analysis for the wave vector \( \mathbf{k}_2 \) indicated in figures 1 and 2. (a) Solid (black) and dotted (red) lines represent the electron polarization (equation (12)) parallel (\( \mathbf{u} = \mathbf{k}_\parallel \)) and perpendicular (\( \mathbf{u} = \mathbf{k}_\perp \)) to the electron wave vector, respectively. The dashed line shows the very small polarization perpendicular to the surface. (b) Spin-projected DOS parallel to the electron momentum, i.e. \( \mathbf{u} = \hat{k}_\parallel \) in \( D^\pm_{\mathbf{k}_\parallel}(\mathbf{k}, \omega) \) and \( D^\mp_{\mathbf{k}_\perp}(\mathbf{k}, \omega) \) (arbitrary units) in equations (10) and (11), (c) same for \( \mathbf{u} = \hat{k}_\perp \), and (d) \( \mathbf{u} = \hat{z} \).

close to 50%. If the polarization direction of \( S_1 \) and \( S_2 \) were perfectly perpendicular to \( \Gamma - \bar{S} \), the contribution of \( S_1 \) and \( S_2 \) to \( D^\pm_{\mathbf{k}_1}(\mathbf{k}, \omega) \) would be exactly zero. This is so because perfect spin polarization for a given direction \( \mathbf{u} \) would imply perfect spin alignment along \( \mathbf{u} \), thus either equation (11) or (10) would give exactly zero. It turns out, however, that the magnitude of polarization is very sensitive to the angle between the magnetization direction and \( \mathbf{u} \). For example, the angle between \( \sigma_{\mathbf{k}_1,S_1} \) and the \( \Gamma - \bar{S} \) line being \( \sim 81^\circ \) (a rather small deviation from \( 90^\circ \)), already gives rise to a non-negligible polarization. In contrast, the dashed (green) line in panels (a) representing the polarization perpendicular to the surface, demonstrates negligible spin polarization. This is also clear from panels (d), where \( D^\pm_{\mathbf{k}_1}(\mathbf{k}, \omega) \) and \( D^\mp_{\mathbf{k}_2}(\mathbf{k}, \omega) \) are almost indistinguishable. All these results are very similar for both considered wave vectors, \( \mathbf{k}_1 \) and \( \mathbf{k}_2 \), with the difference that the states \( S_1 \) and \( S_2 \) are occupied for \( \mathbf{k}_1 \) and unoccupied for \( \mathbf{k}_2 \).

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Figure 6. Surface-projected magnetization \( \langle \hat{\sigma} \rangle_{S_1} \) for the surface state \( S_1 \) as a function of momentum. The solid black line represents the \( S_1 \)-derived Fermi surface sheet. The colour code refers to the magnitude where blue indicates the area where \( \langle \hat{\sigma} \rangle_{S_1} \approx 0 \).

Figures 6 and 7 demonstrate the momentum dependence of the surface-projected magnetization, \( \hat{\sigma}_{k,n} \), for the states \( S_1 \) and \( S_2 \), respectively. The irreducible wedge of the Brillouin zone is indicated by solid lines, whereas the dotted line connects \( \tilde{\Gamma} \) with the \( \tilde{S} \) point. The Fermi surface sheets \( S_1 \) in figure 6 and \( S_2 \) in figure 7 are highlighted by the black colour, whereas all the others are plotted in grey. The shape of the \( S_1 \) and \( S_2 \) bands is similar to three-dimensional paraboloids, inverted around the \( \tilde{S} \) point and with their maximum precisely at \( \tilde{S} \). \( \sigma_{k,n} \) has an almost negligible surface normal component for both states, and at \( E_F \) both the \( S_1 \) and \( S_2 \) surface states are found to be almost perfectly spin polarized (\( |\hat{\sigma}| \approx 1 \)) within the surface plane. The colour code indicates the surface-projected value of the magnetization, \( |\hat{\sigma}_{k,n}| \equiv \sqrt{\sigma^2_{x,k,n} + \sigma^2_{y,k,n}} \), with red and blue denoting the maximum (\( |\hat{\sigma}| \approx 1 \)) and minimum (\( |\hat{\sigma}_{\text{min}}| \approx 0 \)) values, respectively. The projected magnetic moment of the \( S_1 \) state is rather anisotropic through the Brillouin zone with its maximum close to the \( \tilde{\Gamma} \sim \tilde{S} \) direction in the occupied part. Around the Fermi level, the \( S_1 \) state is close to circularly polarized with respect to the \( \tilde{S} \) point and the magnetization is far from being tangential to the Fermi section. Compared with \( S_1 \), the \( S_2 \) state is polarized approximately in opposite direction, and the magnetic moment shows a more pronounced anisotropy, with its maximum close to the \( \tilde{\Gamma} \sim \tilde{S} \) line at the Fermi contour.

An extension of figures 6 and 7 to the rest of the Brillouin zone can be accomplished by considering time-reversal symmetry \( ((k, \sigma) \rightarrow (-k, -\sigma)) \) together with a three-dimensional \( 180^\circ \) rotation around the \( k_x \) and \( k_y \) axes, respectively. The spin-\( \frac{1}{2} \) spinor state rotates according to [30]

\[
S_u = e^{-i(u \cdot \sigma/2)\gamma} = \cos(\gamma/2) \mathbb{I} - i \sin(\gamma/2) u \cdot \sigma
\]

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Figure 7. Surface-projected magnetization $\langle \hat{\sigma} \rangle_{S_2}$ for the surface state $S_2$ as a function of momentum. The solid black line represents the $S_2$-derived Fermi surface sheet. The colour code refers to the magnitude where blue indicates the area where $\langle \hat{\sigma} \rangle_{S_2} \simeq 0$.

finding, for instance, that if one folds figure 6 into the negative $k_x$ area, by a 180° rotation around $u = k_y$, the $x$ component of the magnetization is preserved, whereas the $y$ component changes its sign (unlike an ordinary vector). As a consequence of this special transformation behaviour of spin $\frac{1}{2}$ particles, the absolute value of the magnetization is perfectly symmetric with respect to both axes, but the rotation of the magnetization has the same sign with respect to the four equivalent high-symmetry $\bar{S}$ points in the Brillouin zone (see figure 1).

4. Conclusions

In summary, we have analysed the relativistic electronic structure of the $1 \times 1$ hydrogen covered W(110) surface. The calculated spin-polarized Fermi surface as well as the simulated spin-resolved ARPES spectra show excellent agreement with existing photoemission measurements for selected wave vectors. We have calculated the momentum dependence of the magnetization in a non-collinear manner, obtaining the shape and magnitude of spin polarization within the Brillouin zone. Our calculations confirm that the spin is circularly polarized with respect to the $\bar{S}$ point, for both the $S_1$ and $S_2$ surface states. These theoretical results support and extend the conclusions drawn from spin-polarized ARPES measurements in the $1 \times 1$ hydrogen covered W(110) surface [4].

Acknowledgments

AE appreciates stimulating discussions with Daniel Sanchez-Portal and Istvan Nagy. This work was supported by the Fellow Gipuzkoa program of the Donostia International Physics Center.
(DIPC), the Austrian Science Fund (project number P16227) and the EXC!ITING network funded by the EU (contract number HPRN-CT-2002-00317).

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