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Extracting the Rashba splitting from scanning tunneling microscopy measurements

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ABSTRACT

The Rashba-type spin-splitting found in many two-dimensional electron systems at surfaces is a band splitting in momentum, which is most easily extracted from angular resolved photoemission data. Scanning tunneling microscopy as a real-space resolving technique relies on quasiparticle interference to extract momentum information about the experimental electronic structure. However, the lifted spin degeneracy in the Rashba split bands imposes a selection rule that makes it impossible to extract the Rashba splitting from single scattering events, e.g. scattering from a point defect in STM data. Nevertheless, going beyond single scattering events, the Rashba-type spin splitting can be extracted from STM data, which will be discussed in this review.

1. Introduction

What is known today as the "Rashba effect" has been first described already in 1960 to explain the band structure of certain non-centrosymmetric semiconductors [1]. Later in 1984, Bychkov and Rashba have generalized this concept to two-dimensional electron gases with "lifted spectral degeneracy" [2]. Generally, the Rashba-effect describes the lifting of the spin degeneracy by a sizable spin–orbit interaction due to a broken structural inversion asymmetry. The resulting bands are not only singly degenerate, but each state has a defined spin polarization tangential to a constant energy contour (in the simplest description). This effect has been extensively studied in semiconductor heterojunctions [3]. In 1996, LaShell et al. discovered the Rashba-type spin-splitting in the surface state of Au(1 1 1) [4]. This discovery has made the Rashba effect accessible to surface sensitive techniques, such as angular resolved photoemission spectroscopy and scanning tunneling microscopy. At first, it was speculated that such a splitting may be observed in scanning tunneling spectroscopy data [5], but this statement was heavily debated [6,7]. A few years later, it was shown that for impurity scattering the defined spin polarization introduced by the Rashba Hamiltonian renders some of the incoming and outgoing (scattered) waves orthogonal to each other, so the Rashba effect cannot be observed directly [8]. For an isotropic band, a standing wave pattern is observed, which is the same as if the bands were not Rashba-split at all.

Nevertheless, the STM is not completely blind to the Rashba effect. This short review discusses different means of obtaining information about the Rashba-type spin-splitting from the local density of states measured by STM. Many of the results presented here rely on special circumstances that are present in the specific system under investigation, such as a highly anisotropic band structure or special conditions for scattering events, so that it is difficult to draw far-reaching conclusions about the general applicability of the different methods. Still, as there are a few methods available to extract the Rashba parameters from STM data, one or the other may be applicable to future systems to be studied. They can be summarized under three principle means utilized to observe the Rasha effect. These means are quasiparticle scattering, signatures in the density of states, as well as the application of magnetic fields, which are described in the following.

2. Rashba model

In the simplest model, the Rashba effect in the two-dimensional nearly free electron description is given by the Hamiltonian:

$$H = \frac{p^2}{2m^*} + \alpha_R \left(\hat{z} \times p\right) \cdot \boldsymbol{\sigma} \quad (1)$$

where p is the momentum operator, m^* is the effective mass, α_R is the Rashba coupling constant, $\hat{z}$ is the unit vector in z-direction, which is perpendicular to the plane of the surface, and $\boldsymbol{\sigma}$ is the

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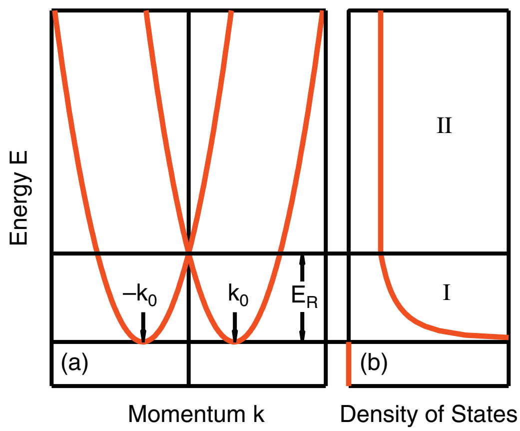

Fig. 1. (a) Parabolic band dispersion of the nearly free electron gas with Rashba-type spin-splitting. The characteristic parameters like the momentum offset k_0 and the Rashba energy E_R are marked. (b) Corresponding density of states with two charactersitic regions. Region I shows a $1/\sqrt{E}$-behavior with a singularity at the band edge. Region II recovers the constant density of states typical for a two-dimensional electron gas.

vector of Pauli matrices. Solving this Hamiltonian within the nearly free electron model, the energy dispersion is given by:

$$E = \frac{\hbar^2 k^2}{2m^*} \pm \alpha_R k \tag{2}$$

where $\hbar$ is the reduced Planck constant and $k = |\mathbf{k}|$ is the electron wave vector. The strength of the spin-splitting is given by the coupling constant α_R, which is the Rashba parameter. It is not directly accessible experimentally. Completing the square in the energy dispersion in Eq. (2) yields:

$$E = \frac{\hbar^2}{2m^*}(k \pm k_0)^2 + \text{const} \tag{3}$$

Here, $k_0 = m^* \alpha_R / \hbar^2$ is the momentum offset, which describes the momentum shift of the split parabolas away from the high symmetry point. The band dispersion is shown in Fig. 1(a) with the characteristic parameters marked accordingly. The momentum offset is an easily observable parameter in angular-resolved photoemission spectroscopy. Projecting the momentum offset onto an energy scale defines the Rashba energy $E_R = \hbar^2 k_0^2 / 2m^*$ [9], which is the energy difference between the band extremum and the crossing point of the two parabolas (i. e. a time-reversal invariant point in the surface Brillouin zone). This definition differs by a factor of 2 from the one given in Ref. [9], because it is taken as the energy difference between two characteristic points in the band structure. All three parameters α_R, k_0, and E_R can be derived from one another. It depends on the specific experimental situation, which of these parameters is most easily accessible.

3. Scattering

Standing wave patterns are typically observed in the local density of states maps measured by means of the differential conductance with the STM at a certain energy (bias voltage). Fourier transforming such patterns into momentum space reveals the momentum transfer q in the scattering processes. What makes it difficult to extract the Rashba splitting from standing wave patterns in the STM is that the scattered waves can be orthogonal so that interference is inhibited. From the Rashba model in the nearly free electron description, the corresponding wave functions $\psi_\pm$ as described by Petersen and Hedegård are [8]:

$$\psi_+ = e^{ikr}\begin{pmatrix} 1 \\ ie^{i\theta_k} \end{pmatrix} \quad \text{and} \quad \psi_- = e^{ikr}\begin{pmatrix} 1 \\ -ie^{i\theta_k} \end{pmatrix} \tag{4}$$

Here, the sign $\pm$ corresponds to the dispersion branch with positive or negative sign in Eq. (2) and θ_k is the angle between the wave vector and the x-axis. For a simple short-range scattering event at a non-magnetic impurity, an incoming and outgoing wave has to be constructed from each dispersion branch resulting in the linear combination of four contributions, which are displayed in Fig. 2(a) [8]:

$$\begin{aligned}
\psi_1^{\text{out}}(r) &= \frac{1}{\sqrt{r}} e^{ik_1 r}\begin{pmatrix} 1 \\ ie^{i\theta} \end{pmatrix} \\
\psi_2^{\text{out}}(r) &= \frac{1}{\sqrt{r}} e^{ik_2 r}\begin{pmatrix} 1 \\ -ie^{i\theta} \end{pmatrix} \\
\psi_3^{\text{in}}(r) &= \frac{1}{\sqrt{r}} e^{ik_3 r}\begin{pmatrix} 1 \\ ie^{i\theta} \end{pmatrix} \\
\psi_4^{\text{in}}(r) &= \frac{1}{\sqrt{r}} e^{ik_4 r}\begin{pmatrix} 1 \\ -ie^{i\theta} \end{pmatrix}
\end{aligned} \tag{5}$$

The resulting wave function $\Psi(r)$ has the form:

$$\Psi(r) = A\psi_1^{\text{out}}(r) + B\psi_2^{\text{out}}(r) + C\psi_3^{\text{in}}(r) + D\psi_4^{\text{in}}(r) \tag{6}$$

which (using $k_2 = -k_3$ and $k_4 = -k_1$) leads to the local density of states $|\Psi(r)|^2$:

$$|\Psi(r)|^2 = \text{const} + \frac{1}{r}\left((A^*D + B^*C)e^{-i(k_3-k_1)r} + \text{c.c.}\right) \tag{7}$$

Only terms with $k_3 - k_1$ appear in the oscillating terms, so that the Rashba splitting cannot be observed in single scattering events. Still, within this simple Rashba model a standing wave pattern should be observed all the way to the band maximum in contrast to what has been shown for the $m_j = 1/2$-state in the Bi/Ag(111) surface alloy [10]. A second look at the same band has revealed standing wave patterns in the region close to the band maximum above the crossing point [11]. For the incoming and outgoing waves the relevant sign change is in the band velocity and not in the wave vector.

Even when the scattering center is magnetic, thereby locally breaking the time-reversal symmetry, it has been shown experimentally that no change in the standing pattern measured by STM has been observed [12]. The experimental findings are supported by simulations based on the Green's function approach, which essentially confirm that backscattering is suppressed. However, the calculations find a clear backscattering signal in a spatially resolved magnetization map suggesting that the backscattering signal should be observable in spin-polarized STM measurements [13]. Similarly, the same should be true for a Kondo impurity as a scattering center as has been proposed more recently [14]. The Rashba effect has been calculated to be observable in the local magnetic density of states around the Kondo impurity. Here as well, spin-polarized STM will be necessary to observe this effect experimentally.

In the case of an anisotropic surface band structure, as it is the case for the Bi surfaces, the standing wave scattering pattern may be very complex albeit reduced by spin orthogonality during scattering [15–17]. While such a pattern may be used to qualitatively confirm a Rashba-type spin-splitting, a quantitative statement about the strength of the spin-splitting is difficult.