Microscopic View on Relativistic Splitting and Spin-Dependent Scattering of Surface States

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Microscopic origin of the spin-orbit splitting of surface states (Rashba effect) is discussed based on *ab initio* calculations of the wave functions for realistic surfaces. The splitting is found to be primarily due to a spin-orbit induced in-plane modification of the wave function, namely, to its effect on the nonrelativistic Hamiltonian [1].

This calls for a microscopic approach to scattering of surface states from defects. Here, we present a wave-functions based method for scattering on a non-magnetic linear defect at a surface with strong spin-orbit interaction [2]. A proof-of-principle calculation for a model crystal potential demonstrates how spin-selective reflection resonances arise in scattering of Rashba-split surface states by an atomic stripe, see figure. Spin-filtering properties of such linear defects are analyzed within an envelope-function formalism for a perturbed surface based on the Rashba Hamiltonian. The continuous Rashba model provides an adequate picture and reveals the essential physics behind the scattering resonance. The spin-dependent reflection suggests a novel mechanism to manipulate spins on the nanoscale.

References

[1] E. E. Krasovskii, *Microscopic origin of the relativistic splitting of surface states*, Phys. Rev. B **90**, 115434 (2014).
[2] I. A. Nechaev and E. E. Krasovskii, *Spin filtering via resonant reflection of relativistic surface states*, Phys. Rev. B **97**, 041407(R) (2018).

Figures

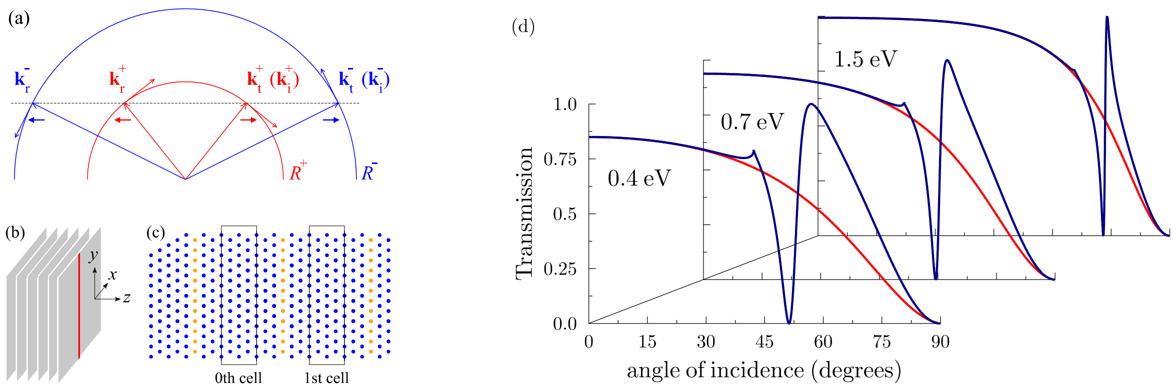

Figure 1. (a) Constant energy contours of Rashba split surface states showing incident, reflected, and transmitted waves. (b) Finite-thickness slab with a linear defect in the topmost layer. (c) Supercell geometry: topmost layer with a repeated row of impurity atoms. (d) Transmission probability as a function of the angle of incidence for $E - E_{\overline{\Gamma}} = 1.5$, 0.7, and 0.4 eV. Red and blue curves are for the incident wave in the inner and in the outer circles, respectively. The latter are seen to be fully reflected at a certain angle depending on the energy.