ELECTRON PARAMAGNETIC RESONANCE OF LOCALIZED SPINS IN TOPOLOGICAL INSULATOR CANDIDATES

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Materials of the family of ternary semiconductors known as Half-Heuslers (HHs) have been shown to be candidates for topological insulators. Recent electron paramagnetic resonance (EPR) experiments [1, 2] in two HHs – YPtBi (topological) and YPdBi (trivial) – slightly doped with magnetic Nd^{3+} impurities have uncovered an intriguing behavior. In YPtBi, the experimental evidence suggests a regime with a strong phonon "bottleneck" effect such that bulk spins relax rather slowly to the lattice and the initial magnetization first diffuses slowly to the surface where coupling to gapless topologically protected surface states finally leads to a quick relaxation process. Motivated by these works, we propose a theoretical description of EPR experiments in Nd-doped Y(Pt/Pd)Bi. For a microscopic description, we first established tight-binding models [3] of the most relevant bands of those compounds. In the case of YPtBi, this allows us to describe the topologically protected surface states. Secondly, we used an Anderson impurity model to couple the magnetic impurities to the surface states. We found that the Kondo coupling constants inherit the exponential spatial dependence of the surface states' envelopes, thus rendering this coupling ineffective within the bulk of the material. In the bulk, on the other hand, spins interact only with gapped states and effectively decouple from the conduction electrons at low temperatures. Based on this, we developed a description of the experimental results by considering the different responses of (a) bulk spins coupled to bulk bands and (b) spins in the surface region coupled to the gapless topological surface states. Using the the Dyson model [4], we adjusted the combined EPR responses of bulk and surface spins to the experimentally determined lines. We found that the larger the bottleneck effect, the stronger the effective contribution of surface spins, thus putting the previous interpretation of the experiments on a firmer theoretical basis.

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