Nonequilibrium spin density in current-carrying topological insulator thin film

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We study microscopic details, over <1 length=“” scale=“” of=“” nonequilibrium=“” spin=“” density=“” s=“” r=“” driven=“” br=“”>by unpolarized charge current injection into a ballistic thin film of Bi₂Se₃ as prototypical topological insulator (TI) material. We find complex nonequilibrium spin texture both on the surfaces of TI and within ~2 nm thick layer near the surfaces because of penetration of evanescent wavefunctions from the metallic surfaces into the bulk. Upon averaging spin texture over few Å, we find large nonzero component of S(r) in the direction transverse to current flow, as well as an order of magnitude smaller out of plane component when momentum of incoming electrons is parallel to the direction of largest hexagonal warping of the Dirac-cone dispersion on the TI surface. Our analysis is based on an extension of the nonequilibrium Green function combined with density functional theory (NEGF+DFT) formalism to situations involving noncollinear spins and spin-orbit coupling. We also demonstrate how DFT calculations with properly optimized local orbital basis set can precisely match putatively more accurate calculations with plane-wave basis set for the supercell of Bi₂Se₃.