Spin selectivity through time-reversal symmetric helical junctions

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Time-reversal symmetric charge and spin transport through a molecule comprising two-orbital channels and connected to two leads is analyzed. It is demonstrated that spin-resolved currents are generated when spin-flip processes are accompanied by a flip of the orbital channels. This surprising finding does not contradict Bardarson's theorem [J. H. Bardarson, J. Phys. A: Math. Theor. 41, 405203 (2008)] for two-terminal junctions: the transmission does possess two pairs of doubly-degenerate eigenvalues as required by the theorem. The spin-filtering effect is explicitly demonstrated for a two-terminal chiral molecular junction, modeled by a two-orbital tight-binding chain with intra-atomic spin-orbit interactions (SOI). In the context of transport through organic molecules like DNA, this effect is termed "chirality-induced spin selectivity" (CISS). The model exhibits spin-splitting without breaking time-reversal symmetry: the intra-atomic SOI induces concomitant spin and orbital flips. Examining these transitions from the point of view of the Bloch states in an infinite molecule, it is shown that they cause shifts in the Bloch wave numbers, of the size of the reciprocal single turn, whose directions depend on the left-and right-handedness of the helix. As a result, spin-up and spin-down states propagate in the opposite directions, leading to the CISS effect. To further substantiate our picture, we present an analytically-tractable expression for the 8×8 scattering matrix of such a (single) molecule.

[1] Yasuhiro Utsumi, Ora Entin-Wohlman, and Amnon Aharony, "Spin selectivity through time-reversal symmetric helical junctions", Phys. Rev. B 102, 035445 (2020)