Breaking Time-Reversal Symmetry and Spin Selection in chiral molecules

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Many recent experiments discovered chiral-induced spin selectivity (CISS): electrons scattered by helical organic molecules become spin-polarized. The theoretical explanation of this phenomenon is still under debate. Many theories start with spin-orbit interactions (SOIs) on the molecule, but the SOI preserves time-reversal symmetry, and therefore implies no spin selectivity in the linear conductance when the molecule connects two single channel terminals (Bardarson's theorem). Here we model the molecule by a tight-binding Hamiltonian, with a Rashba SOI along the helix and additional hopping in the direction of the helix axis, and present several ways to overcome the theorem and achieve CISS: allowing leakage from the molecular ions, adding a third terminal, adding magnetic fields, adding time-dependent potentials, adding more orbital states on the molecule, and various non-linear effects. [1] All of these yield CISS, so we are still far from having a unique explanation. Recent alternative theories will be criticized. [2]

[1] Many relevant references are included in Y. Utsumi, O. Entin-Wohlman, and A. Aharony, Spin selectivity through time-reversal symmetric helical junctions, Phys. Rev. B 102, 035445 (2020) - Editors' suggestion; (arXiv:2005.04041).

[2] O. Enrin-Wohlman, A. Aharony, and Y. Utsumi, Comment on: "Spin-orbit interaction and spin selectivity for tunneling electron transfer in DNA", Phys. Rev. B 103, 077401 (2021); (arXiv:2007.11238).