New frontiers of one step model of photoemission for quantum materials

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Quantum materials feature intertwined electronic correlations, topology, and magnetism, requiring realistic treatments of spin-orbit coupling, interactions, and spin fluctuations. Spin- and time-resolved ARPES (STARPES) is a key probe of their electronic and spin structures, but its quantitative interpretation demands advanced theory. I will present a fully relativistic multiple-scattering Green function (KKR) [1] framework for spin-dependent photoemission that incorporates correlations via DMFT, spin fluctuations via the alloy-analogy model, and light-induced electronic excitations [2,3]. Applications include a one-step photoemission description of altermagnets such as RuO2 and MnTe,where spin-ARPES reveals lifted Kramers degeneracy relevant for spintronics, and kagome magnets such as FeSn thin films, where persistent flat-band splitting and selective band renormalization expose strong correlation and topological effects. This framework provides a unified route to unravel spin dynamics in complex quantum materials [4,5,6,7]. New directions of the photomemission theory in particular the operando ARPES under external perturbations and magnetic fields will be discussed [8].

References:

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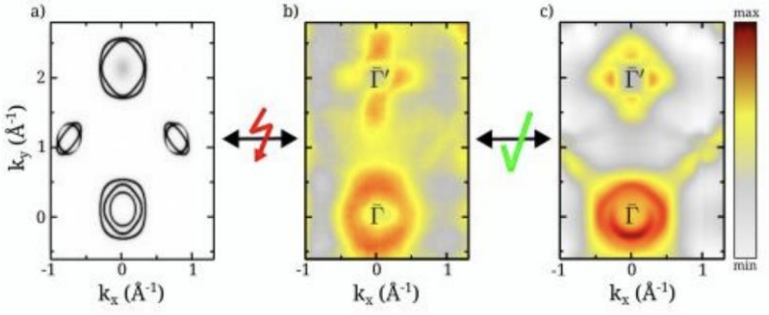

Fermi surface of the high-temperature super-conductor $Ba_{0.6}K_{0.4}Fe_2As_2$ as observed by ARPES (b) and modeled with (a) conventional ground-state theory and (c) advanced one-step photoemission modeling. (G. Derondeau et al. Sci. Rep. **7**, 8787, 2017)