ARPES calculations for highest accuracy

Wolfgang Schattke

Institut fur Theoretische Physik und Astrophysik,Christian-Albrechts-Universitat zu Kiel, Physikzentrum, Leibnizstr. 15, D-24118 Kiel, Germany

Valence band photoemission spectroscopy is theoretically governed by the golden rule which usually is applied at various degrees of accuracy. Here, the one-step model calculation is presented as an ab-initio scheme on an augmented-plane-wave (APW) basis for the initial bound states as well as for the final outgoing states and compared with simplified schemes. Computationally more demanding it shows a significantly higher agreement with experiment. Theory seems to close up with experiment in that detailed effects are revealed and explained through associated spectral structures which nowadays are experimentally resolvable. Thus, a basis is prepared to investigate also next order corrections.

One of the currently most exciting goals in photoemission instrumentation lies in the available modern light sources with high photon intensities. It asks for an extension of photoemission codes towards nonlinear field effects, i.e. the photocurrent beyond quadratic order. Generally speaking, corrections have to be applied to the photoemission vertex in view of higher order diagrams. Ballistic behavior then competes with multiphoton processes if tuned to suitable photon intensity, photon energy and electron detector parameters. The increase of calculation would not be feasible in a straight forward generalization, however, special paths may simplify the task in a first access.