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Correlation, temperature and disorder: recent developments in the one-step description of angle-resolved photoemission

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Abstract

Various apparative developments extended the potential of angle-resolved photoemission spectroscopy tremendously during the last two decades. Modern experimental arrangements consisting of new photon sources, analysers and detectors supply not only extremely high angle and energy resolution but also spin resolution. This provides an adequate platform to study in detail new materials like low-dimensional magnetic structures, Rashba systems, topological insulator materials or high T_C superconductors. The interest in such systems has grown enormously not only because of their technological relevance but even more because of exciting new physics. Furthermore, the use of photon energies from few eV up to several keV makes this experimental technique a rather unique tool to investigate the electronic properties of solids and surfaces.

The following article reviews the corresponding recent theoretical developments in the field of angle-resolved photoemission with a special emphasis on correlation effects, temperature and relativistic aspects. The most successful theoretical approach to deal with angle-resolved photoemission is the so-called spectral function or one-step formulation of the photoemission process. Nowadays, the one-step model allows for photocurrent calculations for photon energies ranging from a few eV to more than 10 keV, to deal with arbitrarily ordered and disordered systems, to account for finite temperatures, and considering in addition strong correlation effects within the dynamical mean-field theory or similar advanced approaches.

Keywords: photoemission, one-step model, correlation, disorder, temperature
PACS: 73.20.-r, 75.70.Rf, 75.50.Bb, 79.60.-i

1. Introduction

Over the past several decades angle-resolved photoemission (ARPES) [1, 2, 3, 4, 5, 6, 7, 8] and inverse photoemission (IPE) [9, 10, 11] have developed into the techniques of choice for determining the occupied as well as the unoccupied electronic structure of any new crystalline material. It is thus in some respects a very mature tool in material science and solid state physics. On the theory side, about 50 years ago photoemission theory appeared as an intractable many-body problem [12, 13, 14, 15]. The first and most simple version of a one-electron approximation for the photocurrent has been given by Berglund and Spicer [16], the so-called three-step model of photoemission. In the framework of this model the photoemission process is artificially divided into three independent steps: the excitation of the photoelectron, its transport through the crystal to the surface and its escape into the vacuum. Self-energy corrections, which represent