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Spectral properties of transition metal pnictides and chalcogenides: Angle-resolved photoemission spectroscopy and dynamical mean-field theory

Les propriétés spectrales des pnictures et chalcogénures de métaux de transition : Photoémission résolue en angle et théorie du champ moyen dynamique

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ABSTRACT

Electronic Coulomb correlations lead to characteristic signatures in the spectroscopy of transition metal pnictides and chalcogenides: quasi-particle renormalizations, lifetime effects or incoherent badly metallic behavior above relatively low coherence temperatures are measures of many-body effects due to local Hubbard and Hund's couplings. We review and compare the results of angle-resolved photoemission spectroscopy experiments (ARPES) and of combined density functional/dynamical mean-field theory (DFT+DMFT) calculations. We emphasize the doping-dependence of the quasi-particle mass renormalization and coherence properties.

RÉSUMÉ

Les corrélations électroniques de Coulomb sont la cause d'empreintes caractéristiques dans les spectres des pnictures et chalcogénures de métaux de transition : la renormalisation de la masse des quasi-particules, la diminution de leur temps de vie ou le comportement de type mauvais métal au-dessus de températures de cohérence relativement basses permettent ainsi d'évaluer les effets des interactions à plusieurs corps dues aux couplages locaux de Hubbard et de Hund. Nous effectuons une revue et une comparaison des résultats expérimentaux de photoémission résolue en angle (ARPES) et des calculs théoriques combinant la théorie de la fonctionnelle de la densité avec la théorie du champ moyen dynamique (DFT+DMFT). Nous insistons en particulier sur la dépendance

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de la renormalisation de la masse des quasi-particules et des propriétés de cohérence en fonction du dopage.

1. Introduction

Angle-resolved photoemission spectroscopy (ARPES) is a powerful tool to probe the electronic properties of materials. It allows for a measurement of the momentum-resolved spectral function, providing crucial information on the Fermi surface, the quasi-particle dispersions, or even the momentum-resolved magnitude of the superconducting gap. It can also give insights into the orbital characters of the electronic states through the use of polarized light, core and plasmon excitations, and some clues about the lifetime of quasiparticles – though the latter point is more delicate since the measurements can be influenced by the sample quality or other extrinsic limitations. In the following, we will focus on measurements in the paramagnetic normal state, except for Section 5 where we summarize recent work on measurements of the superconducting gap.

This review is organized as follows: in Sections 2 and 3 we give brief introductions to the basics of photoemission spectroscopy and dynamical mean field based electronic structure calculations respectively. Section 4 provides an overview over the spectral properties of transition metal pnictide and chalcogenides from a combined experimental and theoretical point of view. Section 5 is devoted to measurements of the superconducting gap, while Section 6 summarizes recent theoretical advances.

2. Angle-resolved photoemission spectroscopy

2.1. Introduction

Photoemission spectroscopy, also called photoelectron spectroscopy, is a technique based on the photoelectric effect [1]. A light source is used to produce photons of a given energy, which are sent on a sample with a chosen incidence. An electron of the sample can then absorb a photon of the incident beam and escape with a maximum energy $E = \hbar\omega - \phi$ with ϕ the workfunction of the material. By collecting those electrons and analyzing their energies and wave vectors, one obtains information about the electronic structure of the material, such as a direct visualization of the quasiparticle dispersions and of the Fermi surface (for a comprehensive book, see, e.g., Ref. [2]; for an introduction, see, e.g., Refs. [3,4]).

The photoemission process is often interpreted within the three-step model, in which the electron is excited from an initial state to a final state, then travels to the surface, and finally escapes from the solid. Fundamentally, the analysis of the photoemission spectrum is a many-body problem, for the escape of an electron leaves the solid in an excited state that may involve several electrons. Another description making use of fewer approximations is the one-step model, in which the photoemission process is described as an optical transition between a ground-state many-body wave function involving N electrons and an excited wave function involving $N-1$ electrons and an escaping plane wave. The photocurrent is described within the sudden approximation, which states that the creation of the photohole is instantaneous and that there is no interaction between the escaped electron and the remaining system. The photocurrent in the three-step model is proportional to the probability of transition between the ground state and all final states. For a given final state it is determined by Fermi's golden rule:

$$w_{\mathrm{fi}} = \frac{2\pi}{\hbar} | < \psi_{\mathrm{f}}^{N} | H^{\mathrm{int}} | \psi_{\mathrm{i}}^{N} > |^2 \delta(E_{\mathrm{f}}^{N} - E_{\mathrm{i}}^{N} - h\nu) \tag{1}$$

In the sudden approximation, $< \psi_{\mathrm{f}}^{N} | H^{\mathrm{int}} | \psi_{\mathrm{i}}^{N} > = < \phi_{\mathrm{f}}^{k} | \tilde{\mathrm{H}}^{\mathrm{int}} | \phi_{\mathrm{i}}^{k} > < \psi_{\mathrm{f}}^{N-1} | c_k | \psi_{\mathrm{i}}^{N} >$, where ϕ^k is a one-electron wave function.

This factorization is valid in the limit of infinite photon energy, and is used as an approximation in practice. It has been argued that the adiabatic to sudden transition takes place at a very large photon energy – of the order of the keV – when many-body effects like core electron - plasmon interaction take place, while smaller energies are required in the case of a localized system (see for instance [6,7]). Still, most of the ARPES experimental analysis is nowadays done within the sudden approximation. For a pedagogical discussion of effects beyond the sudden approximation we refer the reader to Ref. [8]. A DMFT-based approach in the framework of the one-step model has been worked out in Ref. [9].

Summing over all possible excited final states ψ_e^{N-1} with energy E_e^{N-1} and writing $< \phi_{\mathrm{f}}^{k} | \tilde{\mathrm{H}}^{\mathrm{int}} | \phi_{\mathrm{i}}^{k} > = M_{f,i}^{k}$ the one-electron dipole matrix element, we see that the probability of detecting an electron with wave vector k and energy E_{kin} is proportional to:

$$I(k, E_{\mathrm{kin}}) \propto \sum_{f,i} |M_{f,i}^{k}|^2 \sum_{e} | < \psi_e^{N-1} | c_k | \psi_{\mathrm{i}}^{N} > |^2 \delta(E_{\mathrm{kin}} + E_e^{N-1} - E_{\mathrm{i}}^{N} - h\nu) \tag{2}$$