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Accounting for many-body correlation effects in the calculation of the valence band photoelectron emission spectra of ferromagnets

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Abstract

The influence of dynamical correlation effects on the valence band photoelectron emission of ferromagnetic Fe, Co and Ni has been investigated. Angle-resolved as well as angle-integrated valence band photoelectron emission spectra were calculated on the basis of the one-particle Green's function, which was obtained by using the fully relativistic Korringa–Kohn–Rostoker method. The correlation effects have been included in terms of the electronic self-energy which was calculated self-consistently within Dynamical Mean-Field Theory (DMFT). In addition a theoretical approach to calculate high-energy angle-resolved valence band photoelectron emission spectra is presented.
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1. Introduction

Much information on the electronic structure of magnetic solids is gained by valence band photoelectron emission, that in particular allows one to monitor the dispersion of the electronic band structure. However, photoelectron emission spectra are very difficult to interpret without accompanying theoretical calculations. For these in turn, one in general has to solve a corresponding many-electron problem, which is impossible without the use of more or less severe approximations. For materials for which the kinetic energy of the electrons is more important than the Coulomb

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interaction, the most successful first-principles method is the Local (Spin-) Density Approximation (L(S)DA) to the Density Functional Theory (DFT) [1]. In this case the many-body problem is mapped onto a non-interacting system with the effective one-electron exchange-correlation potential replaced by that of the homogeneous electron gas. For the last two decades ab initio calculations of the valence band photoelectron emission spectra of solids based on the LSDA yielded a good basis for the interpretation of experimental spectra, often leading to a quantitative agreement between theoretical and experimental spectra (for a review see Ref. [2] and references therein). The situation is very different when one considers materials showing pronounced correlation effects, in particular since in all calculations the LDA eigen-energies are implicitly interpreted to be the one-particle excitation energies of the system. It is well known that there are two possible sources of error connected with that approach. Firstly, the LDA provides only an approximate expression for the (local) exchange-correlation potential. Secondly, even with the exact exchange-correlation potential at hand, one is left with the problem that there is no known correspondence between the Kohn–Sham eigen-energies and the one-particle excitation energies [3–6].

In principle for an exact description of the excitation energies the corresponding many-body problem has to be dealt with in a more satisfying way leading to a complex and non-local self-energy. Accordingly, DFT-LDA calculations should be supplemented by many-body methods to arrive at a realistic description of the one-particle excitations in correlated systems. To give an example, let us mention the GW approximation [7] which is well suited for the case of insulators and semi-conductors and has also been applied successfully to transition metals [7–10]. Another approach is to consider Hubbard-type models where those Coulomb-interaction terms are included explicitly that are assumed to be treated insufficiently within DFT-LDA. Already the simplest Hartree–Fock-like realization of such an approach called the LDA + U [11] scheme allowed one to improve considerably the description of the optical and magneto-optical spectra of strongly correlated systems (mostly containing rare earth elements [12,13]). The main advantage of the LDA + U scheme is the energy independence of the self-energy which allows one to use only slightly modified standard band structure methods for calculating optical and magneto-optical spectra. On the other hand the scheme works well only for extremely correlated systems, where Coulomb interactions (U) prevail considerably over the kinetic energy (bandwidth W). For moderately correlated systems ($U \approx W$), which applies for most 3d and 5f elements and their compounds, one has to take into account a non-Hermitian energy-dependent self-energy to get a reasonable description of the electronic structure. Nowadays there are several approaches available to deal with this situation. The most advanced one is the Dynamical Mean-Field Theory (DMFT) [14]. DMFT is a successful approach to investigate strongly correlated systems with local Coulomb interactions. It uses the band structure results calculated, for example, within LDA approximation, as input and then missing electronic correlations are introduced by mapping the lattice problem onto an effective single-site problem which is equivalent to an Anderson impurity model [15]. Due to this equivalence a variety of approximative techniques have been used to solve the DMFT equations, such as Iterated Perturbation Theory (IPT) [14,16], Non-Crossing Approximation (NCA) [17,18], numerical techniques like Quantum Monte Carlo simulations (QMC) [19], Exact Diagonalization (ED) [16,20], Numerical Renormalization Group (NRG) [21], or Fluctuation Exchange (FLEX)[22–24]. The DMFT maps lattice models onto quantum impurity models subject to a self-consistency condition in such a way that the many-body problem for the crystal splits into a single-particle impurity problem and a many-body problem of an effective atom. In fact, the DMFT, due to numerical and analytical techniques developed to solve the effective impurity problem [14], is a very efficient and extensively used approximation to get access to the energy-dependent self-energy $\Sigma(\omega)$. At present LDA + DMFT is the only available ab initio computational technique which is able to treat correlated electronic systems close to a Mott–Hubbard MIT (Metal–Insulator Transition), heavy fermions and *f*-electron

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