Theoretical description of photo emission on excited systems

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The alloy analogy model allows to account for the finite temperature of the lattice when calculating the electronic structure of a solid and - based on this - its spectroscopic properties. This approach was already successfully used to include the impact of thermal atom displacements i.e. lattice vibrations reflecting the lattice temperature within angle resolved photo emission calculations on the basis of the one-step model of photoemission [1]. Here we present the use of the alloy analogy model to deal with thermal fluctuations of the magnetic moments reflecting the spin temperature for a magnetically ordered material. Corresponding results for ferromagnetic Fe will be presented that have been obtained on the basis of the local spin density approximation (LSDA) as well as its combination with the dynamical mean field theory (DMFT) [2] together with corresponding experimental results. Sometimes it seems to be sufficient to represent the impact of the pump pulse of a pump-probe experiment by an effective electronic temperature and the corresponding Fermi distribution function allowing for a straight forward application of the one-step model of photoemission in its standard version [3]. As was demonstrated among others by investigations on two-photon photoemission from ferromagnetic materials a more general description of pump-probe experiments can be achieved by extending the one-step model within the framework of the Keldysh non-equilibrium Green function formalism [4]. A combination of this approach with time-dependent density functional theory (TD-DFT) is presented together with first corresponding results that have been obtained on the basis of the LSDA as well as LSDA+DMFT approach.

References

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