

Correlation versus temperature: angle-resolved photoemission in the range between 10 eV and 10 keV

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Recent developments and improvements in the resolution of angle-resolved photoemission experiments in the UPS as well as in the XPS regime require an improved (or revised) theoretical description of the photoemission process in the framework of the one-step model. In particular, the combination of the KKR band structure method with the dynamical mean field theory (DMFT) provides an improved interpretation of photoemission data including all matrix elements effects [1,2]. Here we present a formalism that allows to include lattice vibrations into the one-step model.

In photoemission spectra, typically, two different effects of lattice-vibrations can be observed. First of all, in the UPS regime electron-phonon interaction reflected by “kinks” and related phenomena occur. Here we present a formalism for the calculation of the force-constant tensor within the KKR Green's function method. As a primary information the formalism gives the real-space force-constant tensor. In a next step, from the k-resolved Eliashberg function we can calculate an electron-phonon self-energy and can include this quantity into the photoemission formalism. The method has been applied to angle-resolved photoemission from Ni and is compared to corresponding experimental data [3].

On the other hand for photon energies in the X-ray regime, the phonon-mediated scattering of photoelectrons gives rise to a broadening and to density of states like features in angle-resolved photoemission. Corresponding work on bcc-W is focussed on this effect. So far a simplified Debye-Waller-like treatment is used which leads to a modified single-site scattering matrix. An extension to the more realistic scheme of Larsson and Pendry will be discussed for the fully relativistic case of correlated photoemission.

References

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