Photoemission Spectra of Correlated Materials from First-Principles Theory

F. Aryasetiawan

Lund University, Mathematical Physics, Lund, Sweden

Photoemission spectra of correlated materials are usually studied using the Hubbard model. Within the Hubbard model the spectral function of a typical correlated metal is often characterised by a three-peak structure: a quasiparticle peak around the Fermi level sandwiched by two satellite features, which are the signature of correlations. These satellite features are commonly interpreted as Hubbard bands, understood within an atomic picture as arising from a strong onsite Coulomb interaction. We have studied the spectral functions of $SrVO_3$, a prototype of correlated metals, as well as $SrMoO_3$ using a newly developed first-principles GW+DMFT theory, a hybrid of the GW method and the dynamical mean-field theory (DMFT). Analysis of the results reveals that the satellite features are better understood as collective charge excitations (plasmons) rather than Hubbard bands. We have also studied a model sodium in which the lattice constant is artificially increased to mimic correlation strength. Indeed, the collective plasmon picture also applies until the lattice constant reaches 1.5 the equilibrium value, at which stage the system turns into a Mott-Hubbard insulator. The present study suggests that the simple Hubbard band interpretation may need to be revised by incorporating low-energy plasmons into the picture. While the Hubbard picture is valid for systems with very localised states, the plasmon picture may be more appropriate for systems that exhibit an itinerant character as reflected in the quasiparticle dispersion observed in photoemission experiments

References

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