Extension of photoemission tomography to atomic photoionization

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The quantum-mechanical description of atoms and molecules is based on their electron wave functions, also known as orbitals. A capable tool to identify those electron orbitals of molecule layers on surfaces is photoemission tomography (PT). With Fermi's Golden rule as its mathematical foundation, it is sensitive to the initial state and the final state of the photo electron. Assuming a basic plane wave as the final state, the molecular orbital structure can be represented by a Fourier Transformation (FT) of measured momentum maps. In this fashion, the electronic wave functions of molecular films on interfaces can be extracted [1].

Fermi's Golden rule holds as well for the angular and energy dependent photo emission from atoms in gas phase. In this context, it is called photoionization cross section. We attempt to investigate if the PT might be generalized, in order to describe cross sectional data from literature, measured in the VUV/EUV spectrum.
Therefore, the initially used FT is exchanged by an integral transformation, which serves the spherical symmetry of atoms, rather than the plane symmetry of molecule layers. Additionally, the Coulomb field of the remaining ion must be considered. These two properties are merged into a so-called Coulomb wave function, which is used as the final state. A numerical version of this integral transformation is implemented. Thus, the initial state is not restricted to a distinct model, like hydrogenic orbitals and any model can be applied. We decided for Slater type orbitals. Thereby, photoionization cross section data from s-states of noble gases can be fitted to radial atomic orbitals.

[1] Puschnig, P. et al. (2009). Reconstruction of Molecular Orbital Densities from Photoemission Data. Science (New York, N.Y.). 326. 702-6. doi:10.1126/science.1176105.