Electron/hole lifetimes in simple and noble metals

Table of Contents

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We present a detailed analysis of electron and hole dynamics in bulk metals, and metallic surfaces by means of first−principles many−body calculations. Quasiparticle damping rates are evaluated from the knowledge of the electron self−energy, which we compute within the GW approximation of many−body theory. Inelastic lifetimes are then obtained along various directions of the electron wave vector, with full inclusion of the band structure of the solid. Average lifetimes are also reported, as a function of the electron energy. In the noble metals, a major contribution from d electrons participating in the screening of electron−electron interactions yields electron lifetimes that are above those of electrons in a free−electron gas with the electron density equal to that of valence electrons. While holes in a free−electron gas are known to live shorter than electrons with the same excitation energy, our results indicate that d−holes in noble metals exhibit longer inelastic lifetimes than excited sp−electrons, in agreement with experiment. For the metallic Be (0001) surface we show that the lifetime is strongly influenced by details of the surface band structure. Intraband transitions within the surface state itself, usually ignored in standard Fermi liquid theory, provide 65%−85% of the full electronic contribution. This intraband contribution makes the energy and momentum dependence of γ to be more 2D−like ($\gamma \propto (E_F-E)^{\alpha}$; $\alpha < 2$)
