Real Space Green’s Function Calculations of RIXS\textsuperscript{1} J.J. KAS, J.J. REHR, U. Washington, J.A. SOININEN, U. Helsinki – We present an \textit{ab initio} theory of resonant inelastic x-ray scattering (RIXS) based on the real-space multiple scattering Green’s function (RSGF) formalism and a quasi-boson model Hamiltonian. It is shown that the RIXS spectrum is quasi-local in nature, depending primarily on the Green’s function close to the absorbing site. Based on several assumptions, we derive an approximation to the RIXS spectrum in terms of a convolution of the x-ray absorption and x-ray emission spectra. In addition, quasi-particle self-energy and other many-body effects are calculated using a many-pole model dielectric function, and included via a convolution of the RIXS spectrum with an energy dependent spectral function. Core hole effects are also investigated. The method is implemented in an extension of the RSMS code FEFF90\textsuperscript{2} and illustrated with several examples. Results are found to be in qualitative agreement with experiment.

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\textsuperscript{2}J.J. Rehr et al., Comptes Rendus Phys. \textbf{10}, 548 (2009)

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