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A generalized Sham-Schlüter equation: the link between nonlocality and frequency dependence MATTEO GATTI, European Theoretical Spectroscopy Facility (ETSF) and LSI, Ecole Polytechnique, CNRS-CEA/DSM, F-91128 Palaiseau, France, VALERIO OLEVANO, European Theoretical Spectroscopy Facility (ETSF) and LEPES, CNRS, 25 Avenue des Martyrs, F-38042 Grenoble, France, LUCIA REINING, European Theoretical Spectroscopy Facility (ETSF) and LSI, Ecole Polytechnique, CNRS-CEA/DSM, F-91128 Palaiseau, France, ILYA V. TOKATLY, Lehrstuhl für Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstrasse 7/B2, D-91054 Erlangen, Germany — We present an in principle exact approach to construct effective potentials and kernels for the calculation of electronic spectra. In particular, the potential that yields the spectral function needed to describe photoemission turns out to be dynamical but local and real. Using explicit examples we illustrate how the nonlocality of the physical self-energy is converted into a frequency dependence of the effective potential. We also show that our approach leads to a very short derivation of a kernel that gives a very good description of absorption or energy-loss spectra of a wide range of materials.

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