

Green's Function Approach for Thermodynamic Properties and Spectra of Systems under Extreme Conditions

John J. Rehr, Joshua J. Kas, Tyler D. Blanton, Tun Sheng Tan

University of Washington, Department of Physics, Seattle, WA 98195-1560

We discuss a finite-temperature Green's function approach for calculations of thermodynamic properties and spectra of electronic systems, from normal to extreme conditions. The approach is based on the retarded cumulant Green's function with a cumulant obtained from the GW approximation. Thermodynamic equilibrium quantities and the equation of state are calculated starting from the Galitskii-Migdal-Koltun sum-rule. Exchange and correlation energies and potentials are extracted by subtracting the corresponding independent electron contributions. The approach is illustrated for the homogeneous electron gas over a wide range of densities and temperatures. Extensions for excited states and spectra are also discussed.