Exact conditions and scaling relations in finite temperature density functional theory STEFANO PITTALIS, Free University Berlin, Germany; European Theoretical Spectroscopy Facility (ETSF); University of Missouri-Columbia, USA , C. R. PROETTO[1], A. FLORIS, Free University Berlin, Germany; European Theoretical Spectroscopy Facility (ETSF), A. SANNA, C. BERSIER, E. K. U. GROSS, Free University Berlin, Germany; European Theoretical Spectroscopy Facility (ETSF); Max-Planck-Institut fuer Mikrostrukturphysik, Halle, Germany — Density functional theory is in principle an exact theory of electronic structure, but in practical applications the corresponding functionals need to be approximated. Accurate and efficient approximations may be developed if exact and relevant properties of the density functionals are known and taken into consideration as constraints. In this work, we present rigorous derivations of exact properties, scaling relations and virial theorems for the main quantities of finite temperature density functional theory. The scaling transformation at finite temperature is introduced and its physical meaning and consequences are elucidated.

[1]Permanent address: Centro Atómico Bariloche and Instituto Balseiro, Argentina.

Stefano Pittalis
University of Missouri-Columbia, USA