Finite temperatures in the context of zero Kelvin density functional theory

Mateus B. P. Querne, Daniel Vieira

Centro de Ciências Tecnológicas, Universidade do Estado de Santa Catarina

Density Functional Theory (DFT) [1,2] has become one of the main tools for electronic structure calculations, including applications in Physics, Chemistry and Biology. Since its formulation, DFT has been especially employed in cases with temperature $T = 0$ K. In situations with $T > 0$ K, the implementation of the so-called “Thermal DFT” (thDFT) [3,4] it is commonly performed by using the same exchange and correlation (XC) functionals as $T = 0$ K, so that the development of the XC functionals which includes explicit temperature effects remains not widely explored. In this context, we intend to investigate how XC functionals are affected by temperature, as well as, proposing an alternative formalism to include thermal effects via Kohn-Sham equations. Specifically, as theoretical laboratories, we consider the application of the thDFT formalism to one-dimensional quantum systems. The main motivation for this choice lies in the simplification of the computational treatment, with the possibility, however, of getting conclusions and trends to be followed or confirmed in a future three-dimensional approach. Considering non-interacting and strongly-interacting systems of electrons submitted to a well potential, we present an alternative procedure of including thermal effects in a Kohn-Sham DFT calculation: using the $T = 0$ K formalism, we propose the construction of an effective potential which incorporates, beyond the electronic interaction, the effects of temperature.