Seminar/Talk

A novel approach for strongly correlated systems: geminal-based wavefunction ansätze

Döme Tibor
ETH Zurich

Host: Misha Lemeshko

Almost all of the quantitative approaches to the electronic structure of molecules and materials are based on the orbital model, which includes Hartree-Fock and Kohn-Sham density-functional theory: The wave function becomes a Slater Determinant (SD), describing electrons interacting in a mean-field fashion. Residual errors are usually mitigated by incorporating coupled-cluster methods and perturbation theories. The orbital model is qualitatively incorrect for systems where distinguishing between occupied and unoccupied orbitals is unsuitable, e.g. for complexes of lanthanides and actinides. These systems are dubbed strongly correlated. Even a qualitatively correct description requires multiple SDs. A promising approach uses geminals (two-electron basis functions) as building blocks for the wave function. This talk focuses on the simplest and most successful geminal method: the antisymmetric product of 1-reference-orbital geminals (AP1roG).

Tuesday, February 12, 2019 02:00pm - 03:30pm
Big Seminar room Ground floor / Office Bldg West (I21.EG.101)

This invitation is valid as a ticket for the ISTA Shuttle from and to Heiligenstadt Station.
Please find a schedule of the ISTA Shuttle on our webpage:
https://ista.ac.at/en/campus/how-to-get-here/ The ISTA Shuttle bus is marked ISTA Shuttle (#142) and has the Institute Logo printed on the side.