IST AUSTRIA
Institute of Science and Technology

Physical Sciences Seminar

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

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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

IST Austria Campus Big Seminar room Ground floor / Office Bldg West (I21.EG.101)

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