武汉物数所理论交叉学术交流系列报告

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Relativistic Normal Coupled-cluster Theory of Atomic Dipole Polarizabilities and Electric Dipole Moments

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About the speaker:

Prof. Sahoo got his PhD at Indian institute of Astrophysics in 2006.He was the guest scientist at GSI Germany, Post-Doc at Max-Planck Institute for the Physics of Complex Systems, Germany, Post-Doc and Project Leader at KVI,Netherland.The Awards and honors he got include ***Young international Scientists Fellowship award*** (2010) from the Chinese Academy of Sciences, and ***the CAS President's International Fellowship Initiative (PIFI)*** for 2017. His research focuses on the high precision atomic many-body theory.He has over 100 publications in peer reviewed journals.

Abstract:

Often a sum-over-states approach is employed to determine atomic polarizabilities for high precision studies. Such an approach may be able to give expected accuracies in few atomic systems, especially when the atomic states can be described by an inert gas configuration and one valence electron outside. Again, a variety of hybrid methods such as CI+MBPT are developed to capture the strong correlation effects in atomic systems starting with contracted orbitals due to atomic nuclei. Such an approach is flawed in the many-body theory context as they do not satisfy size-consistent and size extensivity properties of many-body theory. In fact, calculations of electric dipole moments (EDMs) of two-valence atoms using such approaches differ by more than 40% from the results obtained by the relativistic coupled-cluster (RCC) method. The ordinary RCC method also has disadvantages in calculating polarizabilities and EDMs of atomic systems as it involves non-terminating series and accounts for finite contribution from normalization of wave functions. In this talk, I shall discuss a RCC method imposing bi-orthogonal property among the ket and bra states to take care of the short-comings of the ordinary approach, known as normal coupled-cluster theory in the literature, and results for the Cd and Hg atoms will be demonstrated using these methods and compared with the available experimental and other theoretical results to validate our claims.

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