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INFORMATION ENTROPY IN CONFINED ATOMIC SYSTEMS

Statement of the Problem: Since its inception, informational theoretical concepts have flourished as an important tool to explore various physical and chemical systems. These measures quantify the probability distribution of a state of a system in certain complimentary ways. In last ten years appreciable attention was paid to calculate various information quantities like Renyi entropy (R), Shannon entropy (S), Fisher information (I), Onicescu energy (E) and some complexities in numerous model and real systems, as noticed from a vast amount of literature. However, these are mostly designed for the so-called *unconfined*, free systems. Recently some results have been reported in the literature for the confinement of H and He atom inside an impenetrable (hard) and penetrable (soft) spherical enclosure; mostly within the HF realm. Thus, apparently there is a need and scarcity of accurate good-quality methods for information entropy in confinement studies, which can account for the electron correlation effects. In the last few years, our laboratory has engaged in the development of appropriate methods for these systems. This talk will summarize our attempts in this direction. In essence a Kohn-Sham equation has been solved within the broad domain of nonrelativistic density functional theory. This makes use of a work-function-based exchange potential in conjunction with some local (LDA-type) and non-linear, gradient-corrected (Lee-Yang-Parr) correlation energy functional. Accurate eigenvalues and eigenfunctions are obtained by employing a generalized pseudospectral (GPS) method, providing a non-uniform, optimal spatial discretization in position space. Momentum-space solutions are obtained from the Fourier transforms.

Conclusion & Significance: A density functional method has been developed *for the first time*, for information theoretic measures for studying radial confinement of atoms within a spherical enclosure. Accurate results in position and momentum spaces are obtained by GPS method. It works very well for both *ground*, and importantly for *excited* states, for which DFT has an inherent weakness. The effect of correlation energy on confinement is studied in a systematic manner, in low, moderate and strong regions. We have also successfully pursued the so-called relative information, which is connected to the Kullback-Leibler divergence. Comparison with literature is made, wherever possible. In brief, this offers a simple, accurate DFT method for information theoretic measures in confined atoms.

Biography

Amlan K Roy completed his PhD in Theoretical Chemistry from Punjab University, in India. Later he pursued his Post-Doctoral Research in a number of places in North America, such as University of New Brunswick (Fredericton, Canada), University of Kansas (Lawrence, USA), University of California (Los Angeles, USA), University of Florida (Quantum Theory Project). His primary research interest is to develop methods for electronic structure and dynamics of many-electron systems, within the broad domain of density functional framework. Presently he is an Associate Professor at IISER Kolkata. He has published more than seventy research papers and book chapters in reputed journals. He has been serving as a Reviewer in several renowned journals. His biography has been included in 63rd Edition of Marquis Who's Who in America, 2009. In 2012, he has edited a book entitled *"Theoretical and Computational Developments in Modern Density Functional Theory"*.

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