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A DENSITY FUNCTIONAL METHOD FOR QUANTUM CONFINEMENT IN ATOMIC SYSTEMS

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Confinement of an atom inside an impenetrable cavity was first studied in fourth decade of twentieth century. Progress of research on such quantum systems was reviewed several times, recording their importance in both fundamental physics, chemistry and in various engineering branches. It causes substantial changes in the observable properties, such as energy spectrum, transition frequency, transition probability, polarizability, ionization potential, chemical reactivity etc. They have relevance in many different physical situations, e.g., atoms under plasma environment, impurities in crystal lattice and semiconductor materials, trapping of atoms/molecules in zeolite cages or inside an endohedral cobweb of fullerenes, quantum wells, quantum wires, quantum dots and so forth. Furthermore, such models were designed to mimic high pressure environment inside the core of planets. Also, they have contemporary significance in interpreting various astrophysical phenomena and other interesting areas. Density functional theory (DFT) has played a pivotal and unique role for realistic treatment of atoms, molecules, solids, clusters for three decades. Now, it is an indispensable tool for modern electronic structure calculations. The advantage lies in its ability to account for electron correlation effects in a transparent manner keeping the computational cost affordable. As spatial confinement introduces extensive changes in physical and chemical properties of the concerned systems, it is expected to provide a wealth of new information to uncover the physics behind such phenomena. This is a relatively young research area. We report the preliminary theoretical results on such confined atoms within the broad domain of Hohenberg-Kohn-Sham DFT. A non-variational work-function-based potential accounts for the exchange effects accurately, for both ground and excited states, whereas correlation effects are incorporated by employing a simple parametrized local Wigner functional. The non-relativistic KS equation is solved self-consistently by invoking a generalized pseudospectral (GPS) method. This offers a non-uniform optimal spatial grid discretization which provides accurate eigenvalues, wave functions, expectation values and radial densities. The exchange-only results are practically of Hartree-Fock quality and with correlation; these are comparable to some of the very sophisticated and elaborate (such as CI, MCHF) methods available. Obtained results are compared with existing literature data, wherever possible. Furthermore this is extended for information-theoretic measures like Fisher information, Renyi entropy, Tsallis entropy, Shannon entropy and Onicescu energy, in both position and momentum spaces, which may provide a detailed knowledge about diffusion of wave functions, spread of density, localization-delocalization of particle, etc. The momentum-space wave functions are obtained numerically from the Fourier transformation of respective position-space counterpart. A detailed systematic study of these information measures at various confining radius reveals many new interesting features. In essence, a DFT methodology has been presented for information measures in free and confined atoms.

Biography

Amlan K Roy completed his PhD in Theoretical Chemistry from Punjab University, in India. Later, he pursued his Post-doctoral Research at 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 65 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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