

Study of photo-ionization processes using Full Configuration Interaction Quantum Monte Carlo

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The real time Full Configuration Interaction Quantum Monte Carlo (FCIQMC) method has recently been developed to solve the time-dependent Schrödinger equation stochastically and applied to calculate electronic spectra for many-electrons systems [1]. The application of real time FCIQMC is extended here to treat the photo-ionization processes of atoms. The use of full Hilbert space in FCIQMC allows to capture the interplay between two or more electrons in an atom which is important in describing the photo-ionizations processes accurately. One of the main challenges in treating the photo-ionization process is to get accurate descriptions of both the bound and the continuum states for an extensive space of region. We, therefore, have used numerical grid-points as basis obtaining them following the Finite Element Discrete Variable Representation (FE-DVR). In this work, we present the application of FCIQMC in obtaining ground state energies for atoms using the FE-DVR basis and on studying photo-ionization processes thereafter.

References

1. K. Guther, W. Dobrautz, O. Gunnarsson and A. Alavi, *Physical Review Letters* **121** (2018), 056401.