Abstract Submitted
for the DAMOP14 Meeting of
The American Physical Society

Development of a Cartesian sinc DVR basis for single and double ionization[1] JEREMIAH JONES, DAN HAXTON, Lawrence Berkeley National Laboratory — In this investigation, we explore properties of a grid-based representation designed to calculate phenomena involving single and double (auto)ionization. The method employs a powerful representation of the two-electron operator within a basis of sinc functions. It consists of a tensor decomposition of the operator such that two-electron matrix elements may be computed in $O(N^2)$ operations, as opposed to the $O(N^4)$ calculations required for the usual Gaussian basis sets used in quantum chemistry. The basis and methods are tested with the hydrogen atom and H_2^+. Results indicate that, in addition to being more scalable, the technique is more accurate than variational method.

[1]Work supported by USDOE, OBES Chemical Sciences, Geosciences, and Biosciences Division

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Date submitted: 30 Jan 2014 Electronic form version 1.4