



THE UNIVERSITY OF CHICAGO

Departments of Computer Science, Mathematics, Statistics and the Computation Institute
SCIENTIFIC AND STATISTICAL COMPUTING SEMINAR

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Electron Correlation in Van Der Waals Interactions

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226 Jones Laboratory, 5747 S. Ellis Avenue

ABSTRACT

We examine a technique of Slater and Kirkwood which provides an exact resolution of the asymptotic behavior of the van der Waals attraction between two hydrogens atoms. We modify their technique to make the problem more tractable analytically and more easily solvable by numerical methods. Moreover, we prove rigorously that this approach provides an exact solution for the asymptotic electron correlation. The proof makes use of recent results that utilize the Feshbach-Schur perturbation technique. We provide visual representations of the asymptotic electron correlation (entanglement) based on the use of Laguerre approximations. We also describe an a computational approach using the Feshbach-Schur perturbation and tensor-contraction techniques that make a standard finite difference approach tractable.

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