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Calculating Relativistic Atomic and Molecular Properties Using Monte Carlo Methods STEVE ALEXANDER, Southwestern University, R.L. COLDWELL, University of Florida — There are a number of computational methods that can be used to calculate the energies and properties of nonrelativistic atoms and molecules. Fully relativistic calculations of these systems are much less common and more complicated. In part, this is because each relativistic particle generates four coupled components and the presence of negative energy states prohibits the use of most variational techniques. In this talk I will describe how variational Monte Carlo methods can be used to calculate the energy and properties of fully relativistic atoms and molecules. Results for both one electron and two electron systems will be presented.

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