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A new Method for Solving the Three-Dimensional Schroedinger Equation in the Presence of Coulomb Singularities

Solving an effective three-dimensional Schroedinger equation is a key ingredient of computational methods for the calculation of atomic, molecular and solid state properties. However, the presence of Coulomb singularities at the nuclei is a challenge for the convergence of any method. In this contribution a new approach is introduced, which is based on writing the wave function as a product of a function that fulfills the cusp condition at all nuclei and a second function that is expanded in a finite element basis set. This approach is discussed in some detail yielding a variational principle for the second function.

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