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Finite Element Calculations for Molecules with multiple Coulomb Centers

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<p>Efficient and reliable methods to solve effective three dimensional Schroedinger equations are an important ingredient for both density functional as well as Hartree Fock methods used to calculate the properties of molecules and solids. In order to judge the accuracy of popular methods such as using Gaussian basis functions or smooth pseudo potentials it is desirable to use a method that promises to be less basis dependent. Such a method is the finite element method, where the convergence of the wave functions and eigen values can be systemically improved. In combination with using a product ansatz of a function f(r) satisfying the cusp conditions at all nuclei and a smooth function phi(r) for the wave function this provides a method to calculate all electron wave functions. The efficiency of this approach in practice depends crucially on finding a finite element grid which provides enough points where needed but does not “waste “ points where not required. In this contribution results obtained for simple molecules via two and three dimensional calculations are given.In addition the finite element calculations are discussed in some detail.

Level (Hons, MSc,
   PhD, other)?

other

Consider for a student
   award (Yes / No)?

No

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

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