The project progress

Milad H. Mobarhan

March 22, 2013

The final aim of this project is to develop a variational Monte Carlo program which can be used to obtain ground state properties of atoms like He, Be, O, Ne, Si etc. I have so far written a general code, which includes:

- Metropolis algorithm (brute force and important sampling)
- Closed form expressions for orbitals up to 3s orbital, including theirs gradient and laplacian.
- Blocking
- One-body density calculations

I have performed calculation for the ground state energy up to Magnesium, and the results have been correct. The thing that I need to include in my code is a minimization technique. I also have started to write the final report and is almost done with the theory part of it.