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Auxiliary Field Quantum Monte Carlo in Continuum Systems
LUKE SHULENBURGER, RICHARD MARTIN, Department of Physics, Univeristy of Illinois at Urbana-Champaign — The auxiliary field Quantum Monte Carlo method allows Monte Carlo to be performed in any basis. This is accomplished by using the Hubbard-Stratonavich transformation to transform two body interactions into an integral over one body interactions. In practice this method has been difficult to use because while exact, it suffered from a phase problem more severe than the sign problem encountered in Diffusion Monte Carlo. Recent work has suggested a phase free approximation that allows this phase problem to be overcome while sacrificing the exact nature of the method[1]. We have implemented the auxiliary field Quantum Monte Carlo algorithm with the phase free approximation in a plane wave basis. The results of this code for the total energy of jellium and silicon are compared to previous work to assess the accuracy of the method and its approximation. We also discuss results obtained for the energy of jellium with a gap caused by modifying the kinetic energy operator. Results from this study may prove useful in developing more accurate functionals for density functional calculations[2]. We conclude with a brief discussion of the strengths and weaknesses of the auxiliary field method within the phase free approximation.

[1] S. Zhang, and H. Krakauer. Phys. Rev. Lett. **90**, 136401 (2003)

[2] C. Gutle, et. al., Int. J. Quant. Chem. **75**, 885 (1999)

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