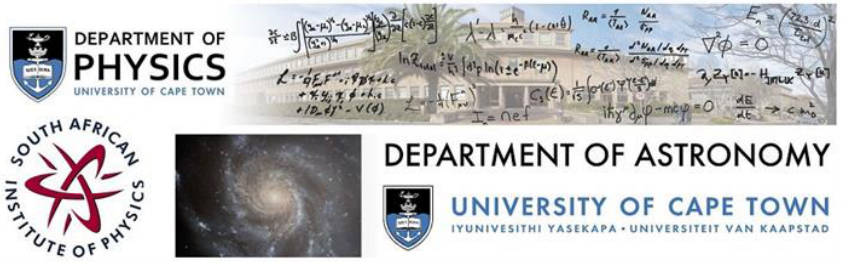

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Density Functional Theory on a Lattice: Self-consistence Hartree plus Exchange Approximation.

Wednesday, 6 July 2016 16:10 (1h 50m)

Abstract content
   (Max 300 words)
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Within an ensemble density functional theory formulation for a finite chain single band Hubbard Hamiltonian we define a 'Hartree plus Exchange' approximation that can be solved exactly in a self-consistent framework. In this formulation we exclude a small 'Correlation' term. Comparison of the results for a short Hubbard chain with the exact values show that the discontinuity in the Kohn-Sham potential is reproduced well and that the approximate total energy is a good approximation of the exact total energy. The results suggest that it is possible to find a good approximate solution for a Hubbard chain of any length and opens the way for solving interesting models such as Hubbard defect chains in a numerically simple and reliable way.

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PhD

Main supervisor (name and email)
and his / her institution

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