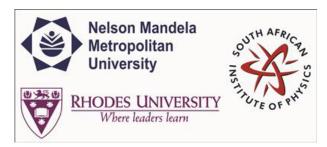
**SAIP2015** 



Contribution ID: 137

Type: Poster Presentation

### Density Functional Theory on a Lattice: Particle Number Dependence of the Exchange-Correlation Potential.

Wednesday, 1 July 2015 16:10 (1h 50m)

# Abstract content <br> &nbsp; (Max 300 words)<br><a href="http://events.saip.org.za/getFile.py/starget="\_blank">Formatting &<br>Special chars</a>

In Kohn-Sham Density Functional Theory, the interacting system is mapped onto a fictitious independent particle system. In an ensemble continuous particle number formulation the exchange-correlation contribution to the potential of the independent particle system has a discontinuity as a function of particle number at integer particle numbers. This discontinuity is equal to the difference between the fundamental gap of the interacting system and the independent particle system. We numerically investigate the exact exchangecorrelation potential as a function of particle number for a finite dimensional Hubbard model and compare the exact results to a local density approximation to the exchange-correlation functional.

#### Apply to be<br> considered for a student <br> &nbsp; award (Yes / No)?

Yes

#### Level for award<br>&nbsp;(Hons, MSc, <br> &nbsp; PhD, N/A)?

PhD

#### Main supervisor (name and email)<br>and his / her institution

Prof. Daniel Joubert

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

Yes

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Session Classification: Poster2

Track Classification: Track G - Theoretical and Computational Physics