Contribution ID: **417** Type: **Oral Presentation**

Particle number dependent discontinuities in density functional derivatives.

Friday, 11 July 2014 11:30 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

The best known particle number dependent discontinuity of a functional derivative in density functional theory is the discontinuity in the exchange-correlation potential, first highlighted by Perdew et al. (Phys. Rev. Lett., 49, 1691, (1982)) and Sham and Schlüter (Phys. Rev. Lett., 51, 1888, 1983)). In this paper it is formally shown that the functional derivatives of the exchange-correlation energy, the interacting kinetic energy, the non-interacting kinetic energy, the mutual Coulomb interaction energy and the correlation part of the kinetic energy can all have spatially independent jumps at integer particle numbers. Formal expressions for the derivative discontinuities are derived and it was shown that the jump exchange-correlation potential can be expressed in terms of a coupling constant integral over the difference in the mutual Coulomb energies of the (J + 1)- and (J - 1)-electron systems.

Apply to be
 considered for a student
   award (Yes / No)?

No

Level for award
 (Hons, MSc,
   PhD)?

N/A

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

No

Primary author: Prof. JOUBERT, Daniel (University of the Witwatersrand)

Presenter: Prof. JOUBERT, Daniel (University of the Witwatersrand)

Session Classification: Theoretical

Track Classification: Track G - Theoretical and Computational Physics