

## **P42 – 2.5-index conditions in a variational density matrix study of the one-dimensional Hubbard model**

Brecht Verstichel

*Department of Physics and Astronomy, Center for Molecular Modeling, Ghent University*

In recent years a lot of research has been aimed at determining the second-order density matrix directly through a variational optimization [Phys. Rev. A 80, 032508 (2009)]. This is an appealing technique because one can determine all ground-state properties without reference to the wave function. The problem is that one has to find N-representability conditions to force the density matrix to be physical, i.e. derivable from a N-particle wave function. We have applied this technique to the one-dimensional Hubbard model and found that the standard two-index conditions are not strong enough in the strong correlation limit below half filling. The three-index conditions, which are computationally much more expensive, are needed to correctly describe this region. In an effort to obtain the same accuracy as with three-index condition, but at the same time keeping the program computationally tractable, we directly determine the three-body density matrix with the third index diagonal. This object contains the necessary three-particle information but all the calculations are still done on two-particle space. We derived new constraints for this object, called the 2.5-index constraints, and found that these get the same level of accuracy as the three-index conditions, while requiring much less computational resources.

