

PHYS

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Tuesday, August 30, 2011

**188 - Nonstandard N-representability constraints and their application to chemical and physical systems***Dimitri Van Neck, Dimitri.VanNeck@UGent.be, Center for Molecular Modelling, Ghent University, Ghent, Belgium B-9052, Belgium*

The accuracy of variationally determined two-body density matrices depends crucially on the N-representability conditions that are imposed. We will discuss some nonstandard types of constraints that can be added to the 2-index constraints to obtain accuracies that are, in some cases, comparable to that obtained by including the computationally much more expensive 3-index conditions. The constraints are illustrated by applications to molecules and to the Hubbard hamiltonian in one and two dimensions.

**Tuesday, August 30, 2011 09:00 AM**[Reduced Density Matrices in Quantum Chemistry and Physics \(08:20 AM - 12:00 PM\)](#)**Location: Colorado Convention Center****Room: 1E**[Close Window](#)