

ABSTRACT: Quantum many-body calculations on parallel machines

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This presentation consists of two topics. First quantum orientational phase transitions in solid hydrogens will be discussed. We have studied a model of coupled quadrupoles via various mean-field approximations and have found evidence for a *reentrant* phase diagram in all isotopes and isotope combinations of hydrogen (H_2 , D_2 , and HD). We are currently working on extending this study to better characterize the behaviour of the solid hydrogens. Second, the total position operator in systems/models with periodic boundary conditions will be discussed. The operator is of the saw-tooth type and satisfies the conditions of Hermiticity, being the generator for total momentum shifts, and its time-derivative gives the current operator. Model calculations are presented in which the operator and its moments are used to distinguish between the metallic and insulating states.