

Abstract Submitted  
for the MAR15 Meeting of  
The American Physical Society

**A Hamiltonian theory of adaptive resolution simulations of classical and quantum models of nuclei** KARSTEN KREIS<sup>1</sup>, DAVIDE DONADIO, KURT KREMER, RAFFAELLO POTESTIO, Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — Quantum delocalization of atomic nuclei strongly affects the physical properties of low temperature systems, such as superfluid helium. However, also at room temperature nuclear quantum effects can play an important role for molecules composed by light atoms. An accurate modeling of these effects is possible making use of the Path Integral formulation of Quantum Mechanics. In simulations, this numerically expensive description can be restricted to a small region of space, while modeling the remaining atoms as classical particles. In this way the computational resources required can be significantly reduced. In the present talk we demonstrate the derivation of a Hamiltonian formulation for a bottom-up, theoretically solid coupling between a classical model and a Path Integral description of the same system. The coupling between the two models is established with the so-called Hamiltonian Adaptive Resolution Scheme, resulting in a fully adaptive setup in which molecules can freely diffuse across the classical and the Path Integral regions by smoothly switching their description on the fly. Finally, we show the validation of the approach by means of adaptive resolution simulations of low temperature parahydrogen.

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Date submitted: 11 Nov 2014

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