

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Molecular Dynamics with Quantum Fluctuations IONUT GEORGESCU, JASON DECKMAN, VLADIMIR MANDELSHTAM, University of California, Irvine — A new Quantum Dynamics approach, called Gaussian Molecular Dynamics (GMD), is introduced. As in the Centroid Molecular Dynamics (CMD), the N-body quantum system is mapped to an N-body classical system with an effective Hamiltonian arising within the Variational Gaussian Wave-packet approximation. The approach is exact for the harmonic oscillator and for the high-temperature limit, accurate in the short time limit and is computationally very efficient. GMD is furthermore used to estimate the diffusion constant and the spectrum of the velocity auto-correlation function of low pressure para-hydrogen at 14K and respectively 25K. The results are consistent with known experimental and theoretical results, such as CMD and RPMD.

Ionut Georgescu
University of California, Irvine

Date submitted: 19 Nov 2010

Electronic form version 1.4