Abstract Submitted
for the SES14 Meeting of
The American Physical Society

Estimation of quantum effects in atomic solids using quantum trajectory dynamics with dissipation[1] BING GU, VITALY RASSOLOV, SOPHYA GARASHCHUK, University of South Carolina, Columbia — We are interested in nuclear quantum-mechanical effects in atomic solids such as helium and para-hydrogen at low temperature. The ground state of these systems is characterized by large zero-point motion of atoms bound to their crystal cites. To make estimates of the zero-point energy (ZPE) given the anharmonicity of the potential and a typical system size of hundreds of atoms, we are developing a methodology based on the quantum trajectories evolving with dissipation. The nuclear wavefunction is represented by an ensemble of quantum trajectories evolving according to the Newtonian equations of motion under the combined influence of the external force, quantum force and friction force [1]. The external potential for solid helium-4 is computed summing up pairwise interactions, and its computation is distributed over multiple ores using Message Passing Interface. The simulation cell for solid helium, which is a $5 \times 3 \times 3$ unit cell in the hexagonal close pack (HCP) form, consists of 180 helium atoms described in Cartesian space i.e. 540 degrees of freedom. The estimated ZPE is estimated from the dynamics of 19200 trajectories. The quantum trajectory dynamics approach will be further used to study a spectrum of chlorine atom trapped in solid He matrices.

[1]NSF CHE-1056188, CHE-1048629, XSEDE TG-DMR110037

Bing Gu
University of South Carolina, Columbia

Date submitted: 19 Sep 2014 Electronic form version 1.4