Atomic Displacements in Quantum Crystals

Marisa Dusseault[1] and Massimo Boninsegni[2]

[1]Memorial University of Newfoundland

[2]Unversity of Alberta

Department of Physics, University of Alberta, Edmonton, Alberta, Canada T6G 2G7

Displacements of atoms and molecules away from lattice sites in helium and parahydrogen solids at low temperature have been studied by means of Quantum Monte Carlo simulations. In the bcc phases of He-3 and He-4, atomic displacements are largely quantum-mechanical in character, even at melting. The computed Lindemann ratio at melting is found to be in good agreement with experimental results for He-4. Unlike the case of helium, in solid parahydrogen there exists near melting a significant thermal contribution to molecular vibrations, accounting for roughly half of the total effect. Although the Lindemann ratio at melting is in quantitative agreement with experiment, computed molecular mean square fluctuations feature a clear temperature dependence, in disagreement with recent experimental observations.