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Developments in the path integral Monte Carlo method for simulating fluids under extreme conditions KENNETH ESLER, University of Illinois at Urbana-Champaign, DAVID CEPERLEY, University of Illinois at Urbana-Champaign — We summarize a number of improvements we have developed for the quantum simulation of fluids under extreme conditions with path integral Monte Carlo (PIMC). PIMC provides way to combine fully-correlated quantum effects with thermal fluctuations in a natural formalism by sampling the many-body thermal density matrix. These developments include the construction of accurate pseudohamiltonians and their incorporation into PIMC, computation of high-accuracy pair density matrices, improved optimization of the long/short-range breakup, a fast embedded band-structure calculation for the fermion nodal restriction, Brillouin-zone integration through twist-averaged boundary conditions, and coupled PIMC/Langevin dynamics. We present preliminary results for the simulation of sodium near its liquid/vapor critical point.

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