

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**Optimization of finite-size errors in finite-temperature calculations of unordered phases** DEEPAK IYER, Bucknell University, MARK SREDNICKI, University of California Santa Barbara, MARCOS RIGOL, Pennsylvania State University — It is common knowledge that the microcanonical, canonical, and grand canonical ensembles are equivalent in thermodynamically large systems. Here, we study finite-size effects in the latter two ensembles. We show that contrary to naive expectations, finite-size errors are exponentially small in grand canonical ensemble calculations of translationally invariant systems in unordered phases at finite temperature. Open boundary conditions and canonical ensemble calculations suffer from finite-size errors that are only polynomially small in the system size. We further show that finite-size effects are generally smallest in numerical linked cluster expansions. Our conclusions are supported by analytical and numerical analyses of classical and quantum systems.

Deepak Iyer  
Bucknell Univ

Date submitted: 27 Oct 2015

Electronic form version 1.4