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Wang-Landau Without Binning G. BROWN, Oak Ridge National Laboratory / Florida State, D. NICHOLSON, KH. ODBADRAKH, M. EISENBACH, A. RUSANU, Oak Ridge National Laboratory — Results are presented for Wang-Landau calculations on a Heisenberg model of BCC Fe that describe the density of states as function defined for all accessible energies instead of a function tabulated at discrete values of the energy. The density of states function described here is an analytic result valid near the ground state supplemented by a polynomial expansion. The probability density of Wang-Landau random walkers is sampled for a fixed density of states, and that probability density can be used to improve the estimated density of states. Methods for evaluating the convergence of the density of states are discussed along with the diffusion behavior of the random walkers. This work was performed at the Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725, and sponsored by the Laboratory Directed Research and Development Program (ORNL), by the Mathematical, Information, and Computational Sciences Division; Office of Advanced Scientific Computing Research (US DOE), and by the Division of Materials Sciences and Engineering; Office of Basic Energy Sciences (US DOE). Computer resources provided by Florida State University.

Gregory Brown
gbrown@fsu.edu
Oak Ridge National Laboratory / Florida State

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