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The Transition Matrix in Flat-histogram Sampling GREGORY BROWN, Florida State University, M. EISENBACH, Y. W. LI, G. M. STOCKS, Oak Ridge National Laboratory, D. M. NICHOLSON, University of North Carolina Asheville, KH. ODBADRAKH, University of Tennessee, P. A. RIKVOLD, Florida State University — Calculating the thermodynamic density of states (DOS) via flat-histogram sampling is a powerful numerical method for characterizing the temperature-dependent properties of materials. Since the calculated DOS is refined directly from the statistics of the sampling, methods of accelerating the sampling, e.g. through windowing and slow forcing, skew the resulting DOS. Calculating the infinite-temperature transition matrix during the flat-histogram sampling decouples the sampling from estimating the DOS, and allows the techniques of Transition Matrix Monte Carlo to be applied. This enables the calculation of the properties for very large system sizes and thus finite-size scaling analysis of the specific heat, magnetic susceptibility, and cumulant crossings at critical points. We discuss these developments in the context of models for magnetocaloric and spin-crossover materials. This work was performed at the Oak Ridge National Laboratory, which is managed by UT-Battelle for the U.S. Department of Energy. It was sponsored by the U.S. Department of Energy, Office of Basic Energy Sciences, Office of Advanced Scientific Computing Research, and the Oak Ridge Leadership Computing Facility. PAR is supported by the National Science Foundation.

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