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Calculating Thermodynamic Properties for Classical and DFT Hamiltonians[1] G. BROWN, Florida State University, D. M. NICHOLSON, M. EISENBACH, ORNL — Using a Gibbs-Bogoliubov approach, the thermodynamic density of states (DOS) for a Hamiltonian can be calculated using that previously determined from the DOS for a similar Hamiltonian. We illustrate this approach for a classical Heisenberg model of bcc Fe by starting from a Hamiltonian that includes up to fourth-neighbor exchange [Tao, et al, J. Appl. Phys. **97**, 10A722 (2005)] and calculating the DOS for a Hamiltonian that includes up to tenth-neighbor exchange. The DOS for this system is calculated using the Wang-Landau method [Wang and Landau, J. Appl. Phys. **97**, 10A722 (2005)] and then compared to the new formalism. The approach can also be used to efficiently calculate the DOS, and hence the thermodynamic properties, for a density-functional theory Hamiltonian starting from classical Heisenberg model.

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