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Exact enumeration of an Ising model for Ni_2MnGa[1] MARKUS EISENBACH, Oak Ridge National Lab, GREGORY BROWN, Florida State Univesity, DON M. NICHOLSON, Oak Ridge National Lab — Exact evaluations of partition functions are generally prohibitively expensive due to exponential growth of phase space with the degrees of freedom. An Ising model with N sites has 2^N possible states, requiring the use of better scaling methods, such as importance sampling Monte-Carlo for all but the smallest systems. Yet the ability to obtain exact solutions for large systems can provide important benchmark results and opportunities for unobscured insight into the underlying physics of the system. Here we present an Ising model for the magnetic sublattices of the important magneto-caloric material Ni_2MnGa and use an exact enumeration algorithm to calculate the number of states $g(E, M_1, M_2)$ for each energy E and sublattice magnetization M_1 and M_2. This allows the efficient calculation of the partition function and derived thermodynamic quantities such as specific heat and susceptibility. Utilizing resources at the Oak Ridge Leadership Facility we are able to calculate $g(E, M_1, M_2)$ for systems of up to 48 sites, which provides important insight into the mechanism for the large magnet-caloric effect in Mn_2NiGa as well as an important benchmark for Monte-Carlo based calculations (esp. Wang-Landau) of $g(E, M_1, M_2)$.

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