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A Performance Comparison of Density-of-States Methods

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Abstract. Nowadays equilibrium thermodynamic properties of materials can be obtained very efficiently by numerical simulations. If the properties are needed over a range of temperatures it is highly efficient to determine the density of states first. For this purpose histogram- and matrix-based methods have been developed. Here we present a performance comparison of a number of those algorithms. The comparison is based on three different benchmarks, which cover systems with discrete and continuous state spaces. For the benchmarks the exact density of states is known, for one benchmark – the FAB system – the exact infinite temperature transition matrix Q is also known. In particular the Wang-Landau algorithm in its standard and $1/t$ variant are compared to Q-methods, where estimates of the infinite temperature transition matrix are obtained by random walks with different acceptance criteria. Overall the Q-matrix methods perform better or at least as good as the histogram methods. In addition, different methods to obtain the density of states from the Q-matrix and their efficiencies are presented.

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1 Introduction

Obtaining the thermodynamic properties of materials is of great importance not only in the science realm but also in many technological application areas like chemical engineering. Apart from an experimental approach, simulations of the material's behavior provide a cost-effective method which avoids potential experimental hazards. One way to perform such a numerical approach is by simulating the material at a fixed temperature or at a number of different temperatures covering the temperature range of interest.

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A more effective way, however, is to determine the density of states (DoS) of the material, because from that all thermodynamic equilibrium properties can be computed based on the partition function and its connection to the free energy.

In order to determine the DoS several numerical algorithms have been developed [1–5]. They can be grouped into histogram-based and matrix-based algorithms. Out of the histogram-based methods we will in particular be concerned with the Wang-Landau algorithm [1, 2, 6–9] and its $1/t$ variant [3, 9, 10]. From the Q-methods which are based on estimating the infinite temperature transition matrix $\boldsymbol{Q}$ we will study the **T**ransition **M**atrix **M**onte **C**arlo (TMMC) method [4, 11, 12] and Q-methods with data collected by the two above mentioned Wang-Landau variants [5, 13]. These methods differ in their numerical effort and precision of the DoS provided, and it seems desirable to compare their performance features.

It is of course clear that the material's properties will have an influence on the performance, and thus one cannot expect to find the one algorithm, which is the best in all cases. Nonetheless, it is certainly very interesting to investigate the performance of the different algorithms on the same material. From such a comparison one might for instance gain some insight into what algorithms provide advantages on certain systems.

Such a broad comparison is unfortunately not available in the literature. However, for the different algorithms of interest here a number of partial performance investigations do exist.

The well studied Wang-Landau method [1, 2, 10] was first presented using an Ising Ferromagnet with no discussion of how the deviation of the density of states from its exact value develops as the algorithm progresses. This was up to later publications, e.g. Shell et al. [14] and Zhou et al. [10]. The latter was also the basis of the Wang-Landau $1/t$ method of Belardinelli et al. [3, 9]. There, extensive studies of both, the standard and $1/t$ variants, were performed and the development of the deviation from the exact DoS with the number of MC steps was analyzed.

The TMMC method is an infinite temperature transition matrix method using the matrix entries as sampling weights. For this method a very thorough study has been conducted by its inventors Wang and Swendsen [12]. The authors investigated several acceptance formulations as well as the multicanonical method and the Wang-Landau method using the Ising Ferromagnet. To calculate the DoS from the transition matrices only the minimization of detailed balance deviations was used, so that unfortunately no comparison with existing eigenvector methods is possible. Also, no comparison of the development of the error in the DoS as a function of MC steps for the different methods was given. Regarding eigenvector calculation for transition matrices, we find a detailed study by Fenwick [15], unfortunately lacking a comparison with the method of minimizing the detailed balance deviations.

Thus it seems fair to say that a thorough comparison between Wang-Landau and transition matrix based methods and combinations thereof is lacking.

In the following we will thus present such a comparison. It will be based on three benchmark systems representing materials with different properties. Particularly well