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Calculation of partition functions by measuring component distributions

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A new algorithm is presented, which allows us to calculate numerically the partition function Z for systems, which can be described by arbitrary interaction graphs and lattices, e.g. Ising models or Potts models (for arbitrary values $q > 0$), including random or diluted models. The new approach is suitable for large systems. The basic idea is to measure the distribution of the number of connected components in the corresponding Fortuin-Kasteleyn representation and to compare with the case of zero degrees of freedom, where the exact result $Z = 1$ is known. As application, $d = 2$ and $d = 3$-dimensional ferromagnetic Potts models are studied, and the critical values q_c, where the transition changes from second to first order, are determined. Large systems of sizes $N = 1000^2$ respectively $N = 100^3$ are treated. The critical value $q_c(d = 2) = 4$ is confirmed and $q_c(d = 3) = 2.35(5)$ is found.

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The partition function is a of fundamental importance in statistical physics [1] and has many applications in other fields like Quantum Mechanics [2], Quantum Field Theory [3], General Relativity [4], Biophysics [5] and Chemistry [6]. Unfortunately only few models are analytically tractable [7]. There is also a fundamental relation to theoretical computer science [8] because obtaining the partition function belongs to the class of NP-hard problems [9], i.e. there is no efficient exact algorithm. Hence, Monte Carlo (MC) simulations [10, 11] are usually applied. The standard approach to obtain the partition function is to measure the free energy by thermodynamic integration of the specific heat, i.e. the fluctuations of the energy. Since this approach is based on measuring fluctuations, it is not very efficient, hence limited to small sizes. One can speedup simulations for certain types of systems by applying cluster algorithms [12–14], multi-histogram methods [15], multicanonical simulations [16, 17] or transition-matrix Monte Carlo [18], but the general problem of the strong fluctuations remains. To overcome this problem, recently Wang and Landau (WL) introduced [19] a simple yet very efficient method to obtain the partition function. The key idea is to measure the density of states by performing a biased random walk in energy space via spin flips. It works well for unfrustrated systems, e.g. the standard q-state Potts model [20], which has become a standard testing ground for Monte Carlo algorithms. The Potts model is of profound interest, because, for dimensions d larger than one, it exhibits order-disorder phase transitions [21], which are of second order for q smaller than a critical value $q_c(d)$, while they are of first order for $q > q_c(d)$. It is analytically proven [22] that $q_c(2) = 4$, but e.g. for $d = 3$, the exact value of q_c is not known. From various analytical work [23–25] and simulations of moderate-size systems [26–28], $2 < q_c(3) < 3$ seems likely. Since the WL method is based on spin flips, it works only for integer values of q, hence the partition function for $2 < q < 3$ cannot be obtained for large systems in this way.

In this letter, an algorithm is presented, which allows us to calculate with high precision numerically the partition function for a large class of systems, e.g. for the q-state Potts models for arbitrary real values $q > 0$. Its partition function is denoted with Z_q here. The approach works for arbitrary interaction graphs, also dilute systems or with random interactions and at any given temperature T. The basic idea is to measure the distribution of the number of connected components in the corresponding Fortuin-Kasteleyn (FK) representation [29] and to compare with the distribution of the case of zero degrees of freedom ($q = 1$), where the exact result $Z_1 = 1$ is known. Large system like $N = 1000^2$ resp. $N = 100^3$ can be treated here, because for the MC simulation, the cluster algorithm of Chayes and Machta [14] is applied. Using this combined approach the critical value $q_c(d = 2) = 4$ is confirmed and $q_c(d = 3) = 2.35(5)$ is found. The outline of the paper is as follows. Next, the model is defined. Then the algorithm for calculating the partition function is presented. In the main part, the results for the $d = 2$ and $d = 3$ Potts models are shown. Finally a summary is given.

The q-state Potts model [20] for integer values of q consists of N spins $\sigma_i \in \{1, \ldots, q\}$ living on the sites of an arbitrary graph or lattice G, with the Hamiltonian $H = -\sum_{(i,j)}(\delta_{\sigma_i,\sigma_j} - 1)$, where the sum runs over the edges (i, j) of G, and δ is the Kronecker delta. For G, here d-dimensional hypercubic lattices of size L having periodic boundary conditions with nearest-neighbor interactions are considered, i.e. $N = L^d$. The partition function $Z_q = \sum_{\{\sigma_i\}} e^{-H/T}$, T being the temperature, can be written in the FK representation [29] as

$$Z_q = \sum_{G' \subset G} W_q(G')$$

$$\equiv \sum_{G'\subset G} p^{N_b(G')}(1-p)^{N_b(G)-N_b(G')} q^{N_c(G')}\,, \quad (1)$$

where the sum runs over all subgraphs of G having the same set of sites and any subset of edges, $W_q(G')$ is the weight of graph G', $p = 1 - e^{-1/T}$, $N_b(G)$ resp. $N_b(G')$ are the number of edges in G resp. G' and $N_c(G')$ is the number of connected components in G'. The FK representation allows for an extension of the model to arbitrary real values of $q > 0$.

For the case of zero degrees of freedom, $q = 1$, we obtain directly $Z_1 = 1$ from the Hamiltonian and the definition of partition function. Note that $W_1(G')$ is the probability of the subgraph G', if the graph is generated randomly by making every edge a member of the subgraph with probability p.

This allows for a calculation of the partition function Z_q for any $q > 0$ in the following way. Let $P_q(c)$ the probability to have c connected components in a subgraph generated according to weight W_q. Then we have by definition

$$\begin{aligned} P_q(c) &\equiv \frac{1}{Z_q}\sum_{G'\subset G} W_q(G')\delta_{N_c(G'),c} \\ &= \frac{1}{Z_q}\sum_{G'\subset G} W_1(G')q^{N_c(G')}\delta_{N_c(G'),c} \\ &= \frac{q^c}{Z_q}\sum_{G'\subset G} W_1(G')\delta_{N_c(G'),c} \\ &= \frac{q^c}{Z_q} Z_1 P_1(c) = \frac{q^c}{Z_q} P_1(c)\,. \end{aligned} \quad (2)$$

Hence, we get

$$Z_q = q^c \frac{P_1(c)}{P_q(c)}\,. \quad (3)$$

This means, by measuring the probability distributions of the number of connected components for random subgraphs ($q = 1$) and for the target value q, we can obtain Z_q. Eq. (3) holds for *all* values of c simultaneously [30]. Therefore, by comparison of the full distributions, one has a means to determine Z_q with very high precision.

Eq. (3) might be useful for analytical calculations, but for most interesting graphs G, the distributions cannot be obtained in this way. Hence, one uses numerical simulations to obtain the distributions $P_1(c)$ and $P_q(c)$. In practice, one can generate random subgraphs directly according to W_1, as explained above, and according to W_q using the very efficient cluster algorithm of Chayes and Machta [14]. This algorithm allows for simulation for arbitrary values of q, similar to other approaches [28, 31, 32].

Nevertheless, for large values of q and finite statistics, $P_1(c)$ and $P_q(c)$ will not overlap, because deviations from the typical value are exponentially suppressed. In this case one has to study intermediate values $q_1, \ldots, q_k \in [1, q]$, calculate each time $P_{q_i}(c)$ and Z_{q_i}. This allows us to extend $P_1(c)$ stepwise [33, 34] for larger values of c, until $P_1(c)$ and $P_q(c)$ have sufficient overlap. In principle, it is a bit ugly, that one has to perform simulations at several values of q_i, but on the other hand, one gets the partition function for all considered values, which will be useful in the following. Note that for the WL algorithm, also one long run is sufficient only in theory. In practice, if the system size is larger than tiny, one has to divide the energy range into intervals, perform independent runs for each interval, and match the results of the different runs as well. In any case, this is no problem for either method, because it can be done automatically by a program, no matter how many intervals have to be matched. The real advantage of the present approach is that it works for all values of $q > 0$, since it does not rely on flips of spins. On the other hand, one must perform simulations for different values of the temperature.

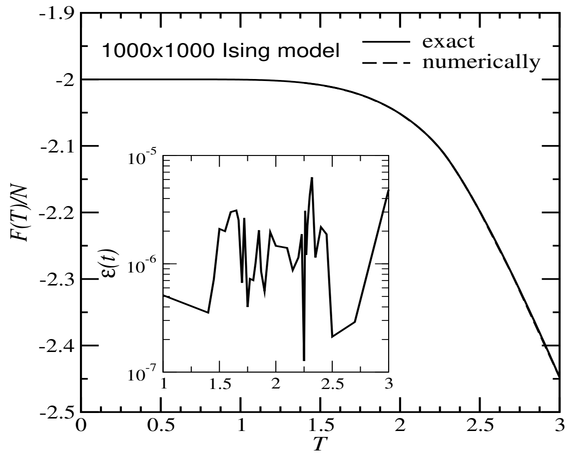

FIG. 1: Free energy F per spin as a function of the temperature T of the two-dimensional Ising model ($q = 2$) obtained by the algorithm and by an exact calculation for system size $L = 1000$. The inset shows the relative error $\epsilon(T)$. For each independent value of temperature, only a total of 5.5×10^5 MC sweeps were performed.

To test the new approach, we now apply it to the two-dimensional Ising model ($q = 2$), where exact results are available for finite system sizes [35]. In Fig. 1, the Gibbs free energy per spin $F/N \equiv -\frac{T}{N}\ln Z_q$ is shown in the Ising representation (i.e. for the Hamiltonian $H = -\sum_{(i,j)}[2\delta_{\sigma_i,\sigma_j} - 1]$). The data of the simulation and the analytical result are given for a large system size $N = 1000 \times 1000$. Thus, $k = 110$ different values q_i are necessary for measuring $P(c)$ over the desired range. Equilibration of the cluster MC simulation is determined by monitoring the number of connected components and the number of edges when starting with a full resp. empty subgraph. Equilibration is assumed when the values for the different starting conditions agree within the range of fluctuations. Due to the global update nature of the

Chayes-Machta algorithm, this is typically the case for few Monte Carlo sweeps. Hence, for each value of q_i, 5×10^3 steps were sufficient to obtain a high accuracy, as shown in the inset of Fig. 1.

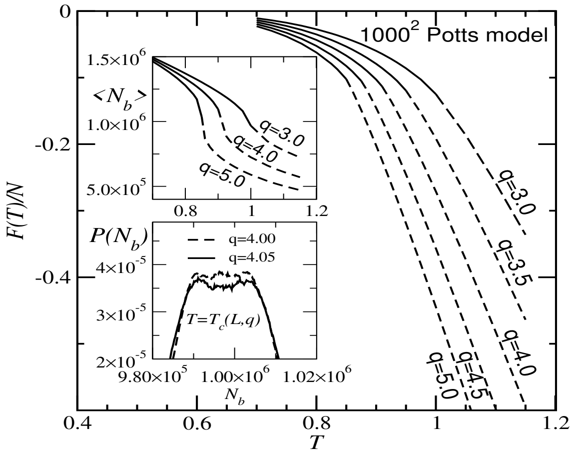

FIG. 2: Free energy per spin of the two-dimensional Potts model ($3 \leq q \leq 5$) for system size $L = 1000$. The upper inset displays the average number of edges N_b as a function of T for $q = 3, 4$ and 5. The lower inset shows the distribution of the number of edges at the temperatures $T(q = 4.00) = 0.910289$ resp. $T(q = 4.05) = 0.906865$.

Since the aim is to determine q_c, the new approach is further tested by applying it to the two-dimensional Potts model, where $q_c = 4$ is known. In Fig. 2, the Gibbs free energy per spin is shown for values in the range $3 \leq q \leq 5$. Due to the large system size, a total of $k = 261$ different values for $q \in [1, 5]$ is necessary. For $q > 4$ a kink at the transition temperatures is visible, as expected. One can calculate derivatives of the free energy analytically from Eq. (1), which allows one to express the mean energy resp. the specific heat by the average number of edges resp. the fluctuations of the number of edges [17, 29], which are available directly from the simulation. The upper inset of Fig. 2 shows the average number $\langle N_b \rangle$ of edges as a function of temperature. One observes that the derivative becomes stronger at the phase transition with growing value of q, almost infinite for $q > 4$, rounded only by finite-size effects, again showing the first-order nature of the transition.

One can determine q_c even more precisely by considering the distribution of the number of edges [26, 28, 36], see lower inset of Fig. 2. The distributions are obtained by performing several long simulations for $T \in [0.906, 0.907]$ resp. $T \in [0.9100, 0.9105]$, exhibiting a total of more than 2×10^7 MC sweeps for each value of q, and combining the results from different temperatures using the multi-histogram approach [15], see also Ref. [10]. For a first order transition, one expects [36, 37] at $T = T_c(L)$ a two-peak structure such that the ratio between maxima and minimum increases with system size. For a second order transition, the ratio stays constant, possibly one. For $q = 4.05$ a two-peak structure is visible, while for $q = 4.00$ not. For smaller sizes $L = 100$ (not shown in the figure), no two-peak structure was found in both cases. This confirms within the given numerical accuracy the known result $q_c = 4$.

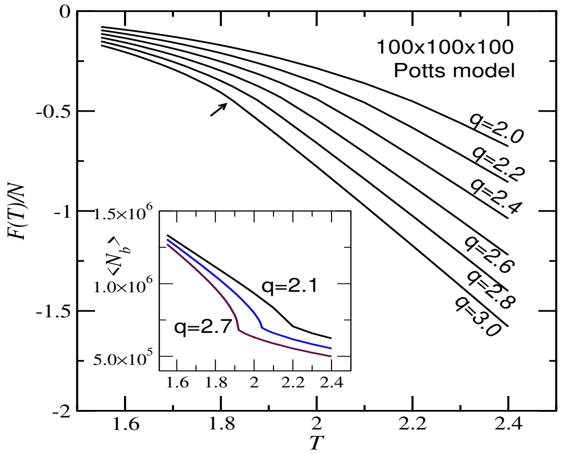

FIG. 3: Free energy F per spin of the three-dimensional Potts model ($2 \leq q \leq 3$) as a function of the temperature T for system size $L = 100$. The arrow indicates the phase transition for $q = 3$. The inset shows the average number of edges N_b as a function of T for $q = 2.1, 2.4$ and 2.7.

For three dimensions, the situation is less clear and no exact analytic results are available. A value of $2 < q_c(3) < 3$ seems likely, see analytical work [23–25] and simulations of moderate-size systems [26–28]. In the range where the transition is first order, the transition seems to be weak, making a direct numerical treatment difficult. This is confirmed by the results for the free energy calculated using the present approach for $N = 100^3$, see Fig. 3. The data is obtained by combining the results for $k = 212$ different values $q_i \in [1, 3]$. No clear kink in any of the functions is visible. Thus, to obtain a precise estimate for q_c, one has to study again the number of edges. The average, shown in the inset of Fig. 3, allows us to see the transition point well, but to infer the order of the transition is still difficult because of finite-size rounding of the curves. The full distributions close to the phase transition are presented in Fig. 4. The distributions are obtained again by performing simulations for several temperatures close to $T_c(L, q)$, for each value of q more than 2×10^6 MC sweeps, and combining the data using the multi-histogram approach [15]. For $q = 2.6, 2.5$ one can see a clear double-peak structure, while for $q = 2.4$ the distribution has only a faint double-peak structure. Just one peak is present for $q = 2.3$. For smaller sizes $N = 20^3$ (not shown), no two-peak structure was found here for $q \leq 2.5$, and only a faint two-peak function for $q = 2.6$. This allows us to conclude $q_c(d = 3) = 2.35(5)$ from the present results, but one cannot exclude an even lower value of q_c.

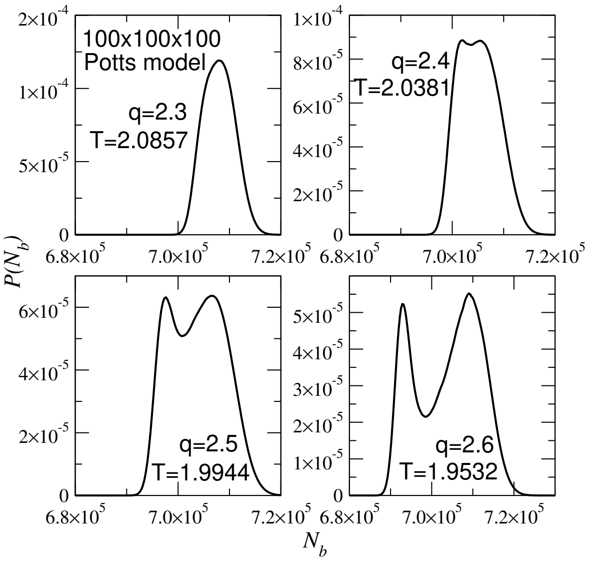

FIG. 4: Distributions of the number of edges at temperature T close to the critical value $T_c(L, q)$ for $q = 2.3, 2.4, 2.5$ and 2.6.

This result is smaller than the result $q_c = 2.620(5)$ obtained by Gliozzi. The deviation is probably due to the fact that in that work much smaller system sizes $N = 14^3$ where used, which shifts the value of q_c up, because slightly above q_c the two-peak structure of $P(N_b)$ becomes visible only for large sizes. The result $q_c = 2.45(10)$ obtained by Lee and Kosterlitz [26] is compatible with our result, although is even less reliable since small sizes were used and data obtained at $q = 3$ was extrapolated to values $q \in [2.7, 3]$. Barkema and de Boer studied [27] a model with integer q, but mimicking the behavior of any $q > 0$, and got $q_c = 2.21$. The results of analytical studies are scattered around the result obtained here: Kogut and Sinclair found [24] $q_c = 2.55$ in a $1/q$ expansion, Nienhuis et al. obtained [23] $q_c \sim 2.2$ using a real-space renormalization approach, while Grollau et al. got [25] $q_c \sim 2.15$ within a Ornstein-Zernicke Approximation.

To summarize, we have introduced a new approach to calculate numerically the partition function of a large class of systems. We present the application to the q-state Potts models for arbitrary values $q > 0$. Using a combination with a fast cluster algorithm we can treat large system sizes. We evaluate the method by performing a comparison with exact analytic results for two-dimensional Ising models of size $N = 1000^2$, and find a very good agreement. For the $d = 2$ Potts model of the same size, we confirm the analytically obtained critical value $q_c = 4$. For the three-dimensional Potts model, due to the weakness of the first order transition, it is hard to infer q_c from the data (size $N = 100^3$) for the free energy. From the analysis of the distribution of the number of edges in the generated subgraphs, we conclude $q_c = 2.35(5)$.

As already mentioned, this approach to obtain the free energy can be applied beyond the standard q-state ferromagnetic Potts model, e.g. for random or diluted ferromagnets, other lattice types and/or higher dimensions, and even arbitrary graphs. The method should work in principle also for frustrated systems, but here the efficient generation of the subgraphs remains an open problem.

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