

Simulations on Infinite-Size Lattices

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We introduce a Monte Carlo method, as a modification of existing cluster algorithms, which allows simulations directly on systems of infinite size, and for quantum models also at $\beta = \infty$. All two-point functions can be obtained, including dynamical information. When the number of iterations is increased, correlation functions at larger distances become available. Limits $q \rightarrow 0$ and $\omega \rightarrow 0$ can be approached directly. As examples we calculate spectra for the $d = 2$ Ising model and for Heisenberg quantum spin ladders with two and four legs.

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Standard Monte Carlo simulations are limited to systems of finite size. Physical results for infinite systems have to be obtained by finite size scaling, assuming that one knows the correct scaling laws and assuming that the data are already in a suitable asymptotic regime. It is therefore very desirable to obtain results also *directly* at infinite system size. We show how to do so, with only a small modification of existing cluster algorithms, by using the cluster representation of the models to calculate two-point functions. In the quantum case we can then also simulate directly at $\beta = \infty$ and calculate correlation functions and dynamical Green's functions. As examples we show calculations for the classical Ising model and for quantum Heisenberg ladder systems.

The *Swendsen-Wang cluster method* [1] for the classical Ising model is based on the Edwards-Sokal-Fortuin-Kasteleyn [2,3] representation

$$e^{\beta J(s_i s_j - 1)} = \sum_{b_{ij}=0,1} p \delta_{s_i s_j} \delta_{b_{ij},1} + (1-p) \delta_{b_{ij},0} \quad (1)$$

$$=: \sum_{b_{ij}=0,1} W_{ij}(s_i, s_j, b_{ij}) \quad (2)$$

for the Boltzmann weight of a spin pair, with $p = 1 - e^{-2\beta J}$, which enlarges the phase space of spin variables s_i by additional bond variables b_{ij} . The partition function $Z = \sum_{\{s_i\}} \sum_{\{b_{ij}\}} W(s, b)$ with total weight $W(s, b) = \prod_{\langle ij \rangle} W_{ij}(s_i, s_j, b_{ij})$ is then simulated efficiently by switching between representations: given a spin configuration $s := \{s_i\}$, one generates a bond configuration $b := \{b_{ij}\}$ with the conditional probability $p(b | s) \sim W(s, b)$, thus creating a configuration of *clusters* of sites connected by bonds $b_{ij} = 1$. Given a bond configuration, a new spin configuration is generated with probability $p(s | b) \sim W(s, b)$. Because of the factor $\delta_{s_i s_j} \delta_{b_{ij},1}$ in W_{ij} , this amounts to setting all spins of each cluster randomly to a common new value, independent of other clusters.

Observables \hat{O} can be computed either in spin representation as $O(s)$ or in bond representation as $O(b) = \sum_s O(s) W(s, b) / \sum_s W(s, b)$ (so called "improved estima-

tors") [4]. For two-point functions $O(s) = s_i s_j$ the bond representation is particularly simple:

$$O(b) = \delta(\text{sites } i \text{ and } j \text{ are in the same cluster}). \quad (3)$$

Thus two-point functions and derived quantities (including susceptibility, energy, and specific heat) can be computed from the properties of individual clusters.

A variant of the Swendsen-Wang method is Wolff's *single cluster method* [4]. Given a spin configuration, only one of the bond clusters is constructed, namely, the cluster which contains a randomly chosen initial starting site x_0 . All spins in this cluster are then flipped. One advantage is that the single cluster will on average be larger than the average Swendsen-Wang cluster, so that its flip results in a bigger move in phase space. Using Eq. (3), the correlation function can then be measured as

$$C(\vec{r}) = \langle s_i s_{i+\vec{r}} \rangle = \left\langle \frac{1}{V_{\text{cl}}} \sum_{i \text{ in cluster}} \delta(i + \vec{r} \text{ in cluster}) \right\rangle, \quad (4)$$

where V_{cl} is the number of sites in the single cluster, and the brackets $\langle \dots \rangle$ on the right refer to the Monte Carlo average. The susceptibility is then $\chi = \beta \langle V_{\text{cl}} \rangle$, the average energy can be measured either as $E = -J2dC(r=1)$, with $r = |\vec{r}|$, or from the average number of bonds in the cluster [2], and the specific heat can be obtained either as a numerical derivative or directly from the bond representation [5].

Our new *infinite system method* now employs the single cluster method, except that it starts each cluster not from a randomly chosen site, but always from the *same* site x_0 (e.g., the origin of the coordinate system). Our method satisfies detailed balance and ergodicity (for any finite region including the origin) similarly to Wolff's method. For the ferromagnetic Ising model, we begin with an initial staggered spin configuration of unlimited size. (Only a finite part of this configuration will have to be stored.) We iterate the following two steps: (i) For the current spin configuration, a cluster containing site x_0 is constructed with Swendsen-Wang bond probabilities and (ii) all spins in this cluster are flipped, resulting in a new spin configuration. The current cluster is discarded after each iteration.

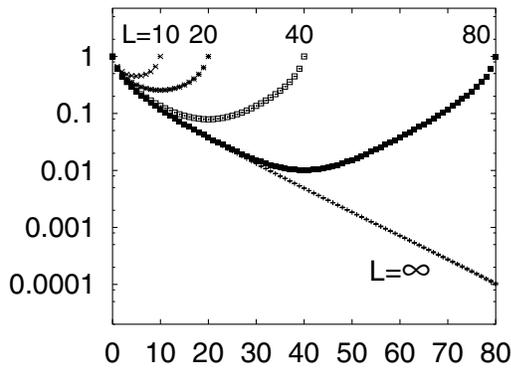


FIG. 1. Correlation functions $C(r)$ vs r of the $d = 2$ Ising model at $\beta = 0.42$.

After a sufficient total number $N(r)$ of iterations, this process will “equilibrate” all spins within a radius r around x_0 , and two-point functions can then be measured within this area. With an increasing number of iterations, the cluster will occasionally reach larger and larger distances. Because of Eq. (4), the probability to do so is (roughly) proportional to the correlation function $C(r)$. A region of the lattice at distance r from x_0 will become “equilibrated” after the cluster has reached that region a sufficient number n_{eq} of times, thus $N(r) \sim \frac{n_{\text{eq}}}{C(r)}$. Since the cluster can grow without bounds, we are calculating correlation functions for the *infinite* lattice, while we only need to store the spin configuration within the area actually reached by a cluster during a finite run.

Figure 1 shows as an example the correlation function for the two dimensional Ising model at $\beta = 0.42 < \beta_c = 0.44068\dots$, calculated according to Eq. (4).

For comparison we show results for finite size lattices, with periodic boundary conditions. Usually, the infinite lattice result can be obtained only as the extrapolation of the finite lattice ones. In contrast, with our new method we can obtain the infinite lattice result in a single simulation, producing the lower straight line in Fig. 1. We checked that the method works just as well in three dimensions.

The calculation of error bars for $C(r)$ needs special care. For each distance $|r|$, we demand that the cluster contains pairs of sites at that distance $|r|^{d-1} \times n_{\text{eq}}$ times; i.e., it reaches each site at that distance $O(n_{\text{eq}})$ [= $O(10)$] times,

before we consider data at that distance thermalized. Only then do we start to accumulate measurements for $C(r)$ according to Eq. (4) for all sites i, j in the cluster. Alternative similar procedures are possible.

Note that the overall computational time is by far dominated by measurements, both in usual cluster algorithms and in our method: In order to obtain a relative error ϵ for $C(r)$, a large number of about $1/\epsilon^2$ clusters with sites at distance r need to occur, each of which is generated with a probability of about $1/C(r)$, in both cases. Thus our method is at least as efficient as usual cluster algorithms, while providing results for the infinite lattice directly.

The average computational time *per cluster* is proportional to the average cluster size, which is proportional to the susceptibility [see below Eq. (4)]. The effective simulated system size grows with the number of iterations.

When will the new method work? The computational effort and thus the susceptibility needs to be finite. In addition, there must not be a finite probability for a percolating cluster, which implies $\beta < \beta_c$. The present implementation of the new method will thus work anywhere in the unbroken phase, right up to the critical point. Systems with long range order may become accessible with a suitable modification of the method. We note that indeed points away from the transition are often the region of interest, when comparing results of simulations to experimental measurements.

For *nonrelativistic quantum systems*, the loop algorithm [6] provides a cluster method. It is based on an enlarged representation in terms of the original spin operators and additional loop operators, similar in spirit to the Edwards-Sokal-Fortuin-Kasteleyn representation, Eq. (1). In the following we specialize on the spin- $\frac{1}{2}$ quantum Heisenberg model

$$\mathcal{H} = J \sum_{\langle ij \rangle} \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) + \lambda S_i^z S_j^z. \quad (5)$$

The two-point function for the single cluster version of the loop algorithm then reads

$$\begin{aligned} \langle \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) \rangle &= \langle \delta(i \text{ and } j \text{ on the loop}) \rangle, \\ \langle S_i^z S_j^z \rangle &= \langle S_i^z S_j^z \delta(i \text{ and } j \text{ on the loop}) \rangle. \end{aligned} \quad (6)$$

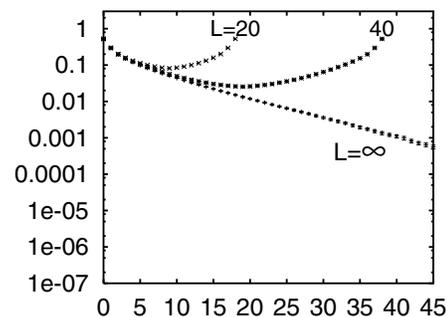
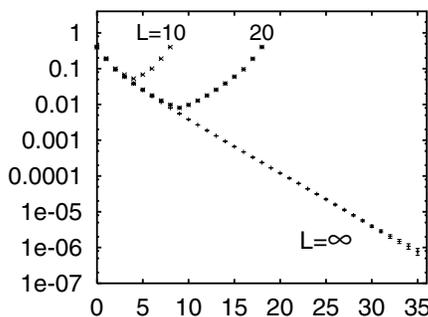


FIG. 2. Equal time staggered spatial correlation function vs distance r , at $q_{\perp} = \pi$ and $\beta = \infty$, for $N = 2$ (left) and $N = 4$ (right).

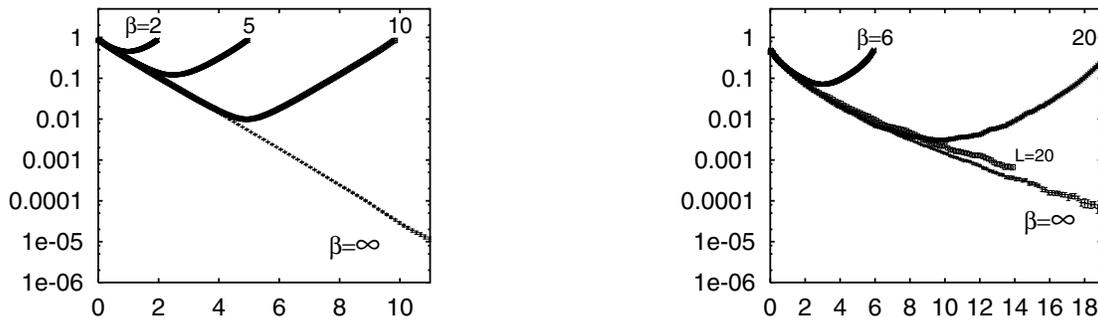


FIG. 3. Green's functions $\langle S(\vec{q}, 0)S(\vec{q}, \tau) \rangle$ vs imaginary time τ , at $\vec{q} = (\pi, \pi)$ for $L = \infty$, the infinite size system, with $N = 2$ (left) and $N = 4$ (right). Results at $L = 20$, $\beta = \infty$ have been added to exemplify finite size effects.

Therefore our approach to simulate infinite size systems can be used in the same way as for the Ising model. "Infinite size" here can be applied to the spatial directions, as well as, independently, to the direction of imaginary time, yielding simulations directly at $\beta = \infty$, while retaining all dynamical information.

Note that our method is not a projector method. We can simulate directly at $L = \infty$ and $\beta = \infty$. This also enables us to obtain the limits $q \rightarrow 0$ and $\omega \rightarrow 0$ directly from the simulations. Contributions from $q \equiv 0$ or $\omega \equiv 0$, which are in general different from those limits and are present in normal simulations with periodic boundary conditions, are completely avoided in our approach, as well as the double limit $L \rightarrow \infty$ and $q \rightarrow 0$ that is usually required. When the number of iterations increases, clusters will reach larger distances in spatial and/or imaginary time direction, thereby improving the resolution in q and ω .

Again, our present method is applicable provided that there is no percolation and that the unsubtracted correlation function drops off sufficiently quickly (i.e., that the corresponding susceptibility is finite).

As an example we studied spin ladder systems [7] with $N = 2$ and 4 legs for the isotropic antiferromagnet ($\lambda = 1$). We used the discrete time version of the loop algorithm ($\Delta\tau = 1/16$). The method can be applied just as well in continuous time [8]. Figure 2 shows results for the equal time staggered spatial correlation functions along the chains, which behave similarly to the Ising case. A fit to the infinite lattice result gives $\xi = 2.93(2)$ for $N = 2$ and $\xi = 8.2(1)$ for $N = 4$. Figure 3 shows Green's functions for $L = \infty$, the infinite size system. Whereas finite temperature calculations give results periodic in imaginary time, which have to be extrapolated, the new approach provides the $\beta = \infty$ ($T = 0$) result directly. With an increased number of iterations, the infinite system results become available at larger distances both in spatial and in imaginary time direction. A fit to the exponential decay $G(\tau) \sim e^{-\tau\Delta}$ of our data directly provides estimates for the gaps $\Delta = 0.5059(4)$ at $N = 2$ and $\Delta = 0.19(1)$ at $N = 4$, consistent with previous results [9]. We also show results for $L = 20$ and $\beta = \infty$ to exemplify the effect of finite size systems.

Continuing the imaginary time Green's function to real frequencies by the maximum entropy method provides the spectra of Fig. 4, in which the gaps, the single magnon peaks, and higher excitations for $N = 4$ are clearly visible. This appears to be the first time that the spectrum for $N = 4$ has been calculated.

Let us compare our method to other approaches. Exact diagonalization provides ground state results but is limited to small systems. Projector methods are also limited in system size and rely critically on proper convergence to the ground state. The Density Matrix Renormalization Group can achieve $\beta = \infty$ (mostly without dynamical information) for fairly small systems, or infinite size for large temperatures and finite $\Delta\tau$. The most powerful method to extrapolate to infinite system size is the finite size scaling method of Kim [10] and Caracciolo *et al.* [11], which allows extrapolation at correlation lengths far larger than the system size but requires knowledge about scaling and corrections to scaling of the model.

In summary, we have introduced a new method, as a small modification of existing cluster methods, to simulate both classical and quantum systems at infinite system size and/or at zero temperature, while obtaining all two-point functions and derived quantities. Larger distances (in space and/or imaginary time) are accessed for longer simulations. The method in its present form is

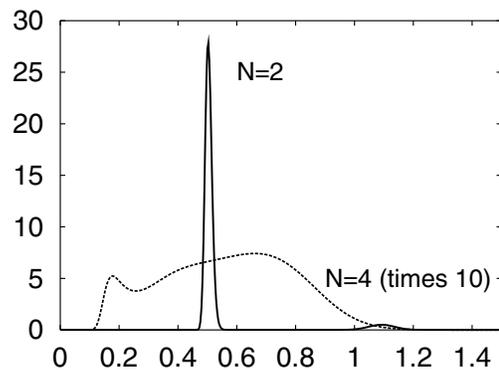


FIG. 4. Spectra $S(\vec{q}, \omega)$ at $\vec{q} = (\pi, \pi)$ for quantum spin ladders with $L = \infty$ and $\beta = \infty$.

applicable to all cases where existing single cluster algorithms can be used, as long as the unsubtracted two-point correlation function decays sufficiently quickly, including any $\beta < \beta_c$ in the unbroken phase. Such points away from a transition are often the region of interest when comparing results of simulations to experimental measurements.

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