Locally converging algorithms for determining the critical temperature in Ising systems

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We introduce a class of algorithms that converge to criticality automatically, in a way similar to the invaded cluster algorithm. Unlike the invaded cluster algorithm which uses global percolation as a test for criticality, these local algorithms use an average over local observables, specifically the number of satisfied bonds, in a feedback loop which drives the system toward criticality. Two specific algorithms are introduced, the average algorithm and the locally converging Wolff algorithm. We apply these algorithms to study the Ising square lattice and the Ising Bethe lattice. We find reasonable convergence to the critical temperature for both systems under the locally converging Wolff algorithm. We also re-examine the phase diagram of the dilute two-dimensional (2D) Ising model and find results supporting our previously reported conclusions regarding the existence of a local regime of magnetization below the percolations threshold. In addition, the presented algorithms are computationally more efficient than the invaded cluster algorithm, requiring less CPU time and memory.

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A useful technique in the computational study of phase transitions in spin systems is the *invaded cluster algorithm* (ICA).[1–5] This algorithm, and others of the same general approach,[6,7] have the property that without prior knowledge of the critical temperature they evolve a spin system to the vicinity of the critical temperature. Let us briefly review the ICA algorithm. Starting in an arbitrary spin state, for example the positive aligned state, the ICA forms one by one a collection of satisfied bonds from the set of all satisfied bonds associated with the spin state. After each bond is added to a cluster, the ICA tests whether this cluster spans the lattice, i.e., has an extent that is of the order of the size of the system. When such a spanning cluster is found, the ICA performs the final step of the Swendsen-Wang (SW) algorithm[8] using this set of clusters. This consists of assigning a random spin value to each of the clusters formed—for the two-state Ising model considered in this paper, this is equivalent to flipping each cluster's spin with probability 1/2.

The SW algorithm relies on the relationship $p(T_c)=1-e^{-2J/k_bT_c}$, established by Fortuin and Kasteleyn,[9] between the critical temperature T_c of the Potts spin lattice with exchange coupling J and the critical bond probability p of the associated (multispecies) bond percolation problem. When the ICA algorithm acts on a spin state typical of $T<T_c$, because the state is relatively ordered, the fraction of satisfied bonds needed to achieve percolation is lower than the fraction needed at a temperature of T_c. Through the Fortuin-Kastelyn relationship, this small fraction of satisfied bonds results in the execution of a SW Monte Carlo step at a high temperature. In a similar way, the ICA generates a large fraction of satisfied bonds when applied to a spin state at $T>T_c$, and so executes a SW step at a temperature $T<T_c$. As the ICA algorithm is repeated, the temperature of the SW steps alternates above and below T_c, rapidly approaching criticality, and finally remains in a narrow range around T_c.

At this temperature the aligned cluster is the smallest that spans the system, and from its density the critical temperature can be inferred. Since the ICA considers the minimal bond density that would globally span the system it can be referred to as a *globally converging algorithm*. Here we wish to introduce *locally converging algorithms* (LCA), where the critical temperature is inferred from local requirements. This is done for the sake of introducing the local algorithms themselves, and also because these algorithms came about from the study of the magnetization regimes in dilute Ising squares.[10] A principal ingredient of these algorithms is the feedback loop, in which results from the current iteration are fed back into the next iteration.

I. INTRODUCTION

Phenomenologically it is known that the ferromagnetic phase transition is characterized by a transition from a zero spontaneous magnetization state to a state with a finite spontaneous magnetization. If we were to observe the details of such a system, quenched from high to low temperature, we would find that after the temperature was lowered, domains of aligned spins started to form and expand. Through a competition between domains of different orientation, and joining of domains with the same orientation, one orientation will become dominant. Effectively, for a given configuration of spins, the ICA selects the highest temperature at which such a dominant domain has formed.

This consideration leads us to the following question regarding the phase transition—when does it become favorable for such an expanding domain to start forming? For consistency it is required that for a system where a dominant domain can form, the answer to the local question above and the corresponding global answer give almost identical results. The word *almost* is used since one can imagine for

example a dilute Ising square lattice with occupation probability slightly greater than the critical occupation probability. In this case global order is possible, but there is a range of temperatures where only local ferromagnetic order exists. We will come back to this system later. The percolation problem in the Bethe lattice[11] provides a playground in which we can better understand the relationship between local characteristics and global order.

A. Exact percolation examples

The main body of this work, following this section, is concerned with the Ising model. In this section two exact examples are given from percolation theory, in order to show in a clear light the local nature of the percolation problem. As was shown by the ICA, the Ising phase transition can be interpreted as a two-species extension of the percolation problem.

1. Bethe lattice

The Bethe lattice is a subset of the Cayley lattice.[11] Since the number of surface elements of the Cayley lattice is proportional to the number of interior sites, taking the thermodynamic limit is a problem, since surface effects cannot be ignored. The Bethe lattice with z nearest neighbors remedies this situation by containing only the interior sites of the corresponding Cayley lattice. Thus all sites of the Bethe lattice are equivalent, sharing z nearest neighbors. Concerns that may be raised include the fact that some of the nearest neighbors of members of the Bethe lattice are not members of the lattice themselves. However, many theoretical arguments and calculations become most clear on this recursive lattice.

Let us see how the percolation problem can be addressed on the Bethe lattice.[11,12] A possible criterion for the percolation threshold is the connectedness of all sites to a border, moving through nearest-neighbor sites. Traveling along such a path, one finds that for a given site on the path there are $z-1$ possible new sites for the next segment in the path, where out of the number of nearest neighbors we have to subtract the direction from which we came. If we denote by p the probability that a given neighbor of the $z-1$ neighbors is occupied, then $p(z-1)$ is the expectation value for the number of new possible branches for the path. Since this process repeats recursively and no loops exist in the lattice, the total number of new branches for a given path would equal the product of the expectation values at each step. Hence, we can identify the critical condition $(z-1)p_c=1$, and the percolation threshold for the Bethe lattice,

$$p_c = \frac{1}{z-1}. \tag{1}$$

More complexity can be introduced to the percolation problem by replacing the lattice points with Ising spins. In this case each site can be empty or occupied, and occupied sites can be in one of two states. The critical percolation condition is that almost all spins, of both orientations, are connected to a border. As was shown by the ICA, the critical percolation condition in this case corresponds to the critical point.

2. Square lattice

In percolation theory, it is known that for the case of the square lattice the bond percolation threshold is 1/2.[11,12] In this subsection we present a heuristic argument for this result with the aid of *unidirectional random walks*.

A unidirectional random walk in two dimensions is a random walk that is restricted to proceed along two perpendicular directions. In two dimensions, from any given site of the lattice we have four equivalent unidirectional walks; i.e., we can choose to take walks only along the $\{\hat{x},\hat{y}\}$, the $\{-\hat{x},\hat{y}\}$, the $\{-\hat{x},-\hat{y}\}$, or the $\{\hat{x},-\hat{y}\}$ directions. Since these are walks to infinity without loops, the percolation threshold is at a maximum 1/2, because we have at least two independent directions in which to proceed at each step. Since all walks have the same starting and end points as these unidirectional walks, and since paths along different choices of perpendicular directions are equivalent up to a rotation—i.e., one unidirectional walk can be obtained by a rotation of the other—there is no other unique route to infinity, besides the single path along an axis, which we can ignore. Hence, 1/2 is the final answer for the percolation threshold.

In three dimensions the problem becomes more difficult. We can form unidirectional walks in a simple cubic lattice by taking walks along any three perpendicular axes; for example, taking the positive x, y, and z axes. Thus, repeating our previous arguments, it would seem that the percolation threshold should be 1/3. However, we must consider that there are paths to infinity that are restricted to a plane formed by two perpendicular axes. Unlike the case of a single path along a single axis, there is an infinite number of such paths in a plane. Note also that paths that are restricted to the plane are not a subset of the paths along three axes. This is because paths along three axes are expected to leave a given plane in a finite number of random steps, whereas paths restricted to a plane are bound to this plane. Thus there are additional possible paths contributing to the bond percolation threshold.

These exact considerations show in a clear light the local nature of the problem of connectedness in the square lattice. For a better understanding of the significance of these considerations to the problem of locally converging algorithms, we add a concept from the study of cluster algorithms[8,13,14]—the *addition probability*.

B. Cluster algorithms

As their name implies, cluster algorithms flip clusters of spins with some probability, instead of the single spins flipped by single-site Monte Carlo algorithms. In the SW algorithm[8] (SWA), the entire sample is divided into clusters, and each of these clusters is flipped with a probability of 1/2. The temperature of the sample is introduced into the algorithm by the probability of adding spins to a cluster, p_a.

Like the SWA, which is at the foundations of the ICA, the Wolff algorithm[14] is a cluster algorithm. Based on the SWA, it was also designed to overcome the critical slowing down of the Metropolis algorithm near the critical point. The difference between the SWA and the Wolff algorithm is that the Wolff algorithm is a local algorithm—selecting a random starting point, setting up a cluster from it, and flipping this

cluster with probability 1. This local property of the Wolff algorithm is the key feature that makes it a useful starting point for locally converging algorithms.

The essence of the Wolff algorithm, and the part that relates it to the temperature, is the building of the cluster to be flipped. This cluster is built by selecting a random seed spin and adding to the cluster satisfied bonds (bonds between aligned spins) with the addition probability, p_a. In order to satisfy the condition of detailed balance one finds that a possibility is to take $p_a=1-e^{-2J}$, with $J=J_0/k_BT$ the effective exchange coupling.[13]

II. LOCALLY CONVERGING ALGORITHMS

The general idea of LCAs can be understood by considering that the conditions for the formation of large clusters of aligned spins are determined by the local characteristics of the system. Hence, in principle it should be possible to determine the threshold probability for the formation of large aligned clusters by considering the local characteristics of the system.

As with the ICA, it is postulated here that for a locally converging algorithm on an Ising lattice the only modification of the condition for percolation is that we consider only satisfied bonds in the count of nearest neighbors. Thus, following the ICA, we introduce the following general plan for a local algorithm:

(1) Start with the system in some state.

(2) Determine the probability threshold for domain expansion by taking a statistical sample of a local quantity.

(3) Do μ Monte Carlo steps with the information obtained in step 2.

(4) Go back to step 2 and repeat.

To see why such an algorithm would converge to the critical point it is enough to repeat the arguments given for the convergence of the ICA. Let us start with all the spins pointing up. In this case step 2 of the above algorithm will give back a critical value of p_a for domain expansion that is less than p_a at criticality, which corresponds to a temperature in the paramagnetic phase. The reason for this is the same as for the ICA. In the all up configuration one needs a lower addition probability to create a large domain (since all bonds are satisfied) which corresponds to a temperature above the critical temperature.[13]

The parameter μ will determine the convergence characteristics of the algorithm. To see this, note if we take a small μ, then the system will go through many iterations of step 2 of the above algorithm on essentially the same configuration. If we pick a μ that is too large, then at each step the sample will converge to the previously chosen temperature, and one can imagine how stable cycles between two temperatures can arise. Both these effects were observed in the numerical data. For the numerical simulation used it was found that taking $\mu=1$ Monte Carlo steps per spin results in good convergence. Note that the ICA uses the determination of the percolation threshold part of the algorithm to generate the set of domains to be flipped, in a way based on the SWA algorithm.[8] In this respect the ICA also performs an equivalent of 1 MCSS between consecutive searches for the percolation thresholds.

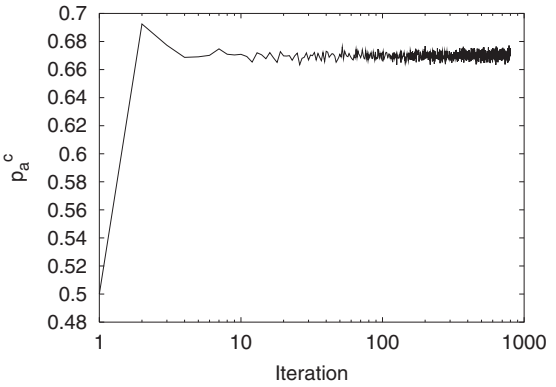

FIG. 1. The average value of Eq. (2) for the Ising Bethe lattice with 17 shells as a function of program time in MCSS. The x axis is given in logarithmic scale so that initial relaxation can be observed.

As the local algorithm is repeated it seeks the lowest probability where a percolating cluster has the potential for growing. Unlike the ICA, which uses a global check for the lowest addition probability for a percolating cluster, a local algorithm seeks a local average for the lowest addition probability where a percolating cluster can potentially form. Since a percolating cluster would need a lower (than critical) addition probability to grow in the ferromagnetic phase, and a higher addition probability to grow in the paramagnetic phase, the local algorithm goes through a feedback loop that converges to the vicinity of the critical addition probability. Note that we use helical boundary conditions for the following calculations.

A. Average algorithm

With this general plan we can design a simple local algorithm for the Bethe lattice where any nearest neighbor is considered to be in an independent direction, orthogonal to any other direction. For the Bethe lattice, since all sites are equivalent and no loops exist, to get to infinity from any given site on the lattice we can repeat the arguments given above with bonds replaced by satisfied bonds. This will lead to an equation similar to Eq. (1) with z replaced by z_s, the number of satisfied bonds,

$$p_a^c = \frac{1}{(z_s - 1)}. \tag{2}$$

We can perform step 2 in the above plan by taking an average of Eq. (2) over all possible spins in the Bethe lattice. The size of the Bethe lattice can be measured in the number of shells it contains. A shell is a collection of spins added in the same iteration. If one were to draw a Cayley lattice, starting from the generator (shell zero), and creating a tree structure of spins below it, a shell would correspond to a horizontal line of spins. Note that the Bethe lattice contains one less shell than the Cayley lattice by construction. Results for such a Bethe lattice with $z=3$ and 17 shells are given in Fig. 1.

To create a numerical model for the Bethe lattice a structure definition[15] is used. Each member of this structure (a site) carries information about its current orientation (zero if

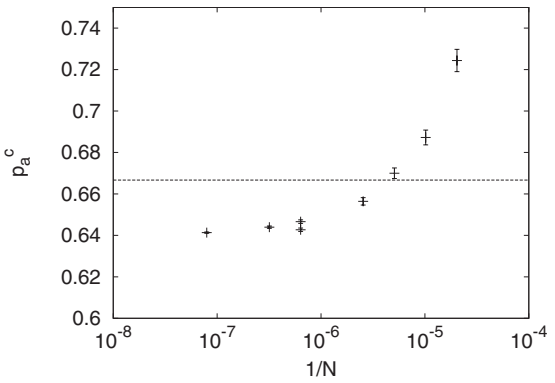

FIG. 2. The average value of the average of Eq. (2) for the Bethe lattice as a function of the inverse of the total number of spins in the lattice. The line at $p_a^c=2/3$ corresponds to the exact result for the Bethe lattice.

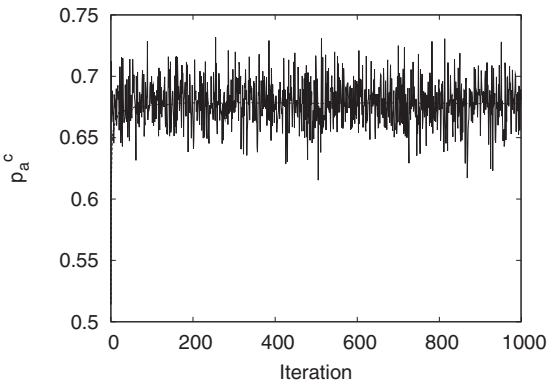

FIG. 3. Relaxation of the critical addition probability for the Bethe lattice with 17 shells produced from the LCWA as a function of the iteration step.

it is empty), and the coordinates of its nearest neighbors. Such a construction is useful also for other lattices because it allows for direct access to the coordinates of the nearest neighbors, with a single calculation at the beginning of the simulation. These calculations for the coordinates of the nearest neighbors typically consume a considerable amount of CPU time, especially in the case of periodic boundary conditions or other boundary conditions that require a check of the calculated coordinate of a neighbor.

Starting from a lattice with all spins pointing up, Eq. (2) is averaged over all sites that have a chance to be on a path to the boundary, i.e., with $z_s \geq 2$, and 1 MCSS of the Metropolis algorithm is simulated. This process is repeated on the order of a thousand times. The result for the critical addition probability as a function of simulation time is given in Fig. 1. We see the critical addition probability converging to the vicinity of the known result for this case, $p_a^c=\frac{2}{3}$. In Fig. 1 the x axis is set to the logarithmic scale so that the rapid relaxation of p_a^c can be observed. Figure 2 gives results for the critical addition probability as a function of $1/N$ with N the number of spins of the lattice. Typically an order of 5% difference is observed between the exact result of 2/3 and the results produced from this model. This error is suspected to result mainly from counting many isolated clusters of spins when taking the average of Eq. (2) and counting only spins with $z_s \geq 2$.

B. Locally converging Wolff algorithm

Let us consider the behavior of the Wolff algorithm in the paramagnetic and ferromagnetic phases. In the paramagnetic phase, since $p_a < p_a^c$ and the system is disordered, only small clusters would form. In the ferromagnetic phase, since $p_a > p_a^c$ and the system is ordered, large clusters would form. We can recognize the critical temperature and the corresponding critical addition probability as those values where such Wolff clusters would barely grow.

We now have a method for performing the local algorithm. Steps 2 and 3 from the general plan described above are combined together, and the determination of the critical addition probability is tied to the Wolff algorithm. Since the version of the Wolff algorithm used[13] flips each spin after its nearest-neighbor spins have been considered, at each step of the algorithm where a spin is considered, only bonds to nonconsidered spins would appear in the number of satisfied bonds z_s'. Hence, for each spin added to the cluster with $z_s' \geq 1$, $p_a=1/z_s'$ is calculated, and the result is averaged for the cluster being built. This ensures that the addition probability will be such that the cluster will barely form. (Note that for the average algorithm, where considered bonds were not erased, we had to subtract the excessive bond explicitly.) The averaged addition probability calculated while the Wolff cluster is grown, is then fed back as the addition probability for the next step in the locally converging Wolff algorithm (LCWA).

Another way to see why this algorithm works is to consider what will happen in the two phases. In a paramagnetic configuration, where the system is disordered, on the average there will be fewer satisfied bonds than at criticality and the returned p_a will be higher than the critical p_a. On the other hand, in a ferromagnetic configuration, where the system is ordered, there will be more satisfied bonds on the average and the returned p_a will be lower than the critical p_a. In such a way the system will be driven toward criticality.

As mentioned earlier, we would like to take the average over the largest clusters. In the process of a Wolff simulation, especially when the system is disordered, some small clusters will form and should not be counted in the average. Also, we would like to have a statistical sample of such clusters from which to take an average. This is achieved by conducting a series of Wolff steps, sorting the clusters in order of cluster diameter, and performing the average over a number of the largest clusters. The results depend very little on the number of clusters over which the average is taken.

Results for the critical addition probability, p_a^c, on the Bethe lattice with three nearest neighbors and 17 shells are presented in Fig. 3. We see a rapid convergence of the system toward the equilibrium point, and small fluctuations around this value. In Fig. 4 the dependence of p_a^c on $1/N$ is given. From these results it is approximated that $p_a^c \approx 0.68$ for the infinite system, in comparison to the exact result, $p_a^c=2/3$.

Results for the critical addition probability, p_a^c, on the square lattice with $L=200$ are presented in Fig. 5. We again

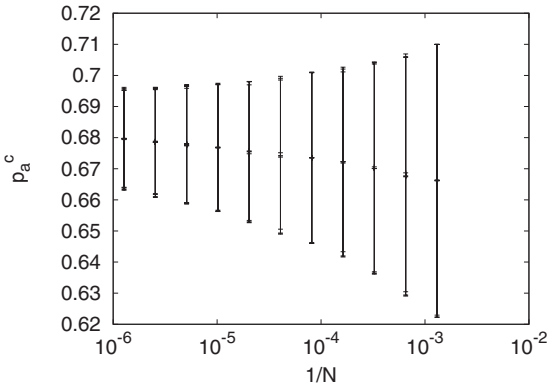

FIG. 4. Average critical addition probability for the Bethe lattice produced by the LCWA as a function of the inverse number of spins. The error bars give the average standard deviation on the tail of a single run. Five runs are given in the plot.

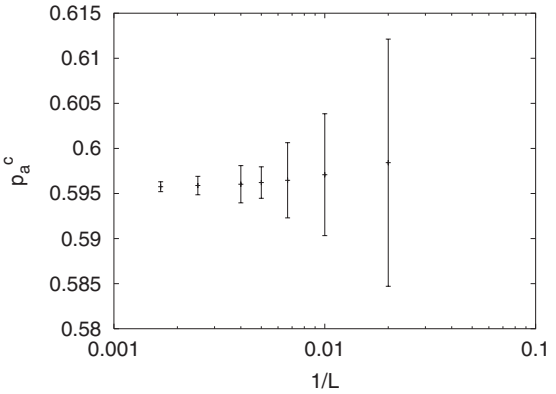

FIG. 6. Average critical addition probability for the square lattice produced by the LCWA as a function of the inverse of the length of the lattice. The error bars give the average standard deviation on the tail of a single run.

see a rapid relaxation of the system toward an equilibrium point, and small fluctuations around this value. In Fig. 6 the dependence of p_a^c on $1/L$ is given. From this data it is approximated that $p_a^c \approx 0.595$ for the infinite system, in comparison to the exact result, $p_a^c \approx 0.5858$.

In both the Bethe lattice and the square lattice the error in p_a^c is less than 2%. In the cases presented here, the last in first out[13] version of the algorithm is used in the creation of the cluster. One should note that different averaging or different versions of the Wolff algorithm may result in a more accurate calculation of the critical point. One should also note that boundary effects tend to increase p_a^c, since at the boundaries in general there are fewer nearest neighbors.

C. The site-dilute Ising surface

We have also applied the LCWA to the site-dilute Ising system[10,16–19] which is homogeneous only statistically. This system provides considerable information about the behavior of ferromagnetic systems in rarefied conditions which are important for many applications such as magnetic memory. As pointed out in a previous publication,[10] this system admits a state of ordered local islands of spins below the percolation threshold, and such systems exhibit cooperative ferromagnetic phenomena, e.g., hysteresis. The LCWA, as a local search for the critical temperature, is naturally suited for dilute systems.

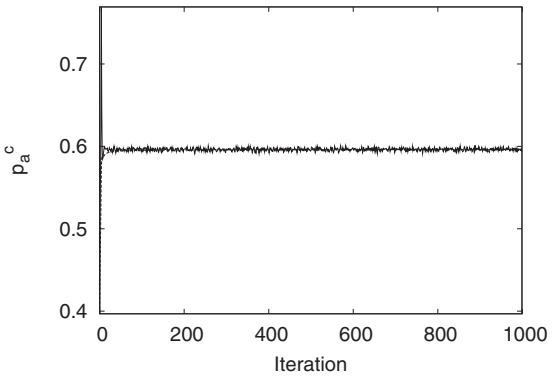

FIG. 5. Relaxation of the critical addition probability for the square lattice with $L=200$ produced from the LCWA as a function of the iteration step.

In Fig. 7 we reproduce parts of Fig. 8 of Ref. 10 for the magnetic regimes in the density-temperature plane of the Ising system. In the figure we also include two calculations of the critical temperature using the LCWA. IC corresponds to the invaded cluster algorithm, SM corresponds to the spontaneous magnetization condition, and HC corresponds to the maximization of the heat capacity. Please see Ref. 10 for more information about these calculations. The calculations of the critical temperature are labeled RARE and FULL, and they refer to two versions of the LCWA. In the FULL case all aligned spins are added to the Wolff cluster as in the first in first out procedure.[13] In the RARE case the cluster is diluted by removing the last addition to it. Three regimes are designated in the figure: (PM) paramagnetism, (LFM) local ferro-

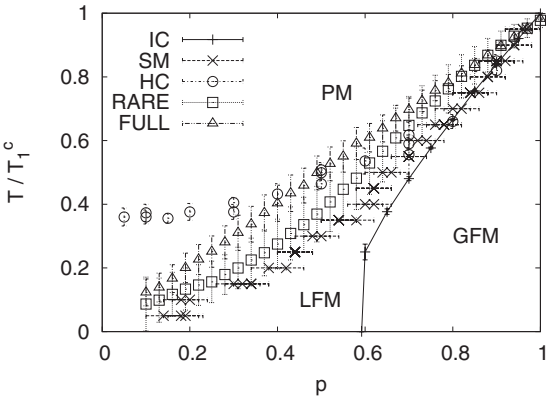

FIG. 7. Magnetic phase diagram as a function of the density and temperature of a 100×100 Ising surface. IC corresponds to the invaded cluster algorithm, SM corresponds to the spontaneous magnetization condition, and HC corresponds to the maximization of the heat capacity. RARE and FULL refer to two versions of the LCWA. In the FULL case all aligned spins are added to the Wolff cluster as in the first in first out procedure (Ref. 13). In the RARE case the cluster is diluted by removing the last addition to it. Three regimes are designated in the figure: paramagnetism, local ferromagnetism, and global ferromagnetism.

magnetism, and (GFM) global ferromagnetism.

We see close agreement between the LCWA and the ICA for the higher densities. As the density is lowered these two algorithms give differing results, with the LCW predicting a higher critical temperature for a given density. This difference widens as one approaches the percolation threshold, past which the LCWA gives finite critical temperatures for the local ferromagnetic regime. This can be understood as follows. While the ICA requires order across the entire lattice, the LCWA permits local ferromagnetic regions that are disconnected. Since order in a ferromagnetic system is monotonically dependent on the temperature, more order requires a lower temperature and hence the widening difference in the critical temperatures. As one passes the percolation threshold with decreasing density, global order is no longer possible for any temperature, while local order is possible at any finite density. Based on previous results[10] the RARE calculation fits better than the FULL one with the curve for spontaneous magnetization. The best approaches for building the clusters for the dilute system are under current investigation.

III. SUMMARY

Algorithms converging automatically to the vicinity of the critical point of Ising systems were introduced. These algorithms use only the local characteristics of the system in the feedback loop that generates convergence. Specifically, two algorithms were introduced, the average algorithm and the LCWA. The average algorithm uses the approach of averaging the local critical addition probabilities of the lattice sites and is appropriate for use when no loops exist in the lattice, such as for the Bethe lattice. The LCWA employs a similar strategy, but utilizes the Wolff algorithm cluster building process to carry out the average. The LCWA was found to be consistently better than the average algorithm for the determination of the critical point. Both algorithms were slightly less accurate in determining the critical point as compared to the ICA, probably due to the more effective sampling technique of the ICA. However, the local algorithms are useful in investigating the occurrence of locally ordered clusters, which is an interesting problem in dilute, and more generally, inhomogeneous systems.

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