



STATISTICAL MECHANICS AND DISORDERED SYSTEMS

Since computers are able to simulate the equilibrium properties of model systems, they may also prove useful for solving the hard optimization problems that arise in the engineering of complex systems.

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The central problem of statistical mechanics is the calculation of the thermodynamic properties of macroscopic systems from the microscopic laws governing the individual atoms or molecules. We might wish to know, for example, how the volume of a fluid will respond to a change in temperature or pressure, or how the magnetization of a crystal will respond to a magnetic field. Calculations of this kind are difficult, however, because of the large number of particles in any real system. When there are 10^{23} variables, there is no way the microscopic equations can be integrated analytically. Moreover, experimental information about the states of systems is extremely sparse. We can measure the temperature and pressure of a gas, but we can never determine the position and velocity of each molecule.

Under these conditions, even the statement of a problem is essentially probabilistic. We want to predict the most probable value of some observable quantity, as well as the fluctuations about this value. Fortunately, the fluctuations of most properties are generally orders of magnitude smaller than we can measure, so that predicted behavior effectively resembles deterministic laws.

Microscopic interactions are extremely short ranged. Each atom or molecule is directly affected only by its neighbors over distances of a few angstroms. Ordered phases, such as crystals, which can be coherent on a length scale of meters, are the result of cooperative effects whereby long-range correlations are established exclusively through short-range interactions. The nature of these correlations differs from material to material, and also for a given substance under different conditions. Water can exist as a gas, liquid, or solid, depending on the pressure and temperature; iron has a

permanent magnetic moment at low temperatures, but is demagnetized above a certain critical temperature.

As the critical temperature is approached, correlations extend over long distances. The characteristic correlation length ξ diverges at the critical temperature as long-range order sets in. In general, the correlation length diverges as a power law with a critical exponent ν :

$$\xi \sim (T - T_c)^{-\nu}. \quad (1)$$

Other thermodynamic properties such as specific heat also exhibit power law singularities:

$$C \propto (T - T_c)^{-\alpha}. \quad (2)$$

An understanding of phase transitions is one of the major accomplishments of condensed matter physics in the last decade [11, 12]. With this understanding comes the ability to derive the associated power law phenomena from simple symmetry arguments.

Considering the nature of the problem, it is natural that numerical methods should play a major role in modern statistical mechanics. One of the most fruitful approaches has been the use of computer simulations. This approach has increased in importance in recent years with the development of powerful methods of analysis for extracting information from the data and with the continued improvement in the capacity of modern computers.

A SIMPLE MODEL

To illustrate current methods, we use a simplified model of a magnet, known as the Ising model, in which the atomic magnetic moments or *spins* are arranged on a lattice and can point only up or down. The microscopic state of the system can be completely specified

by giving the value +1 (up) or -1 (down) to variables s assigned to each lattice site i . Interactions between spins can only occur with the nearest neighbors on the lattice. Neighboring spins have a lower energy ($-J$) if they are pointing in the same direction than if they are pointing in opposite directions ($+J$). For two spins, the interaction energy is

$$E = -Js_1s_2. \quad (3)$$

If a system of two spins is at temperature T , the probability of finding it in the state $\{s_1, s_2\}$ is

$$P(s_1, s_2) = Z^{-1} \exp(-Ks_1s_2), \quad (4)$$

where K is equal to $-J/kT$, k the Boltzmann constant, T the absolute temperature, and Z a normalization factor:

$$Z = 2 \exp(K) + 2 \exp(-K). \quad (5)$$

At high temperatures, K is small and the spins are almost independent. For low temperatures, K is large and it is more probable that the spins will be found in the same state.

To generalize to many spins, we define the Hamiltonian,

$$H = K \sum_{i,j} s_i s_j = KS, \quad (6)$$

where the sum is over nearest neighbors on the lattice. The probability of the state $\{s\}$ is

$$P\{s\} = Z^{-1} \exp(-H), \quad (7)$$

and the normalization factor (known as the partition function) is given by the trace sum over all states $\{s\}$:

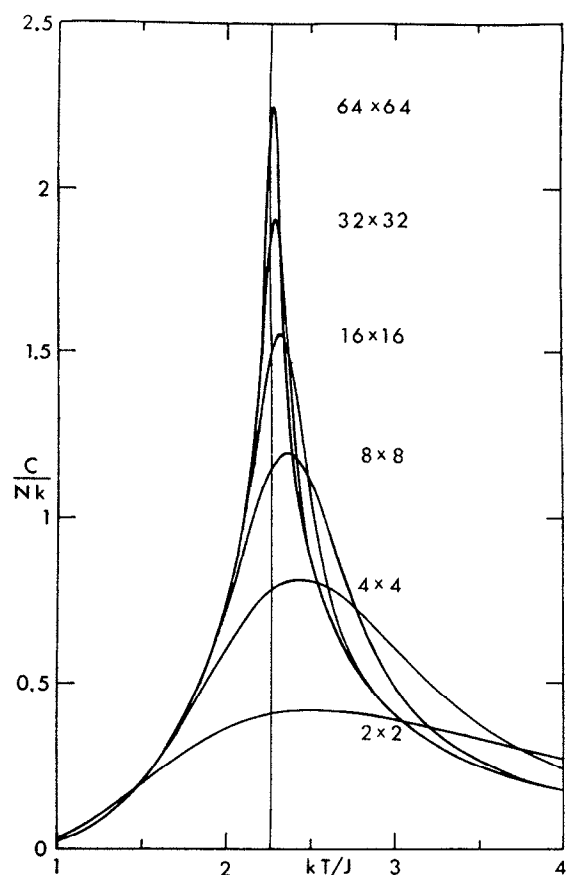
$$Z = \text{Tr}_{\{s\}} \exp(-H). \quad (8)$$

An array of spins on a lattice in two or more dimensions exhibits a phase transition. At high temperatures the correlations between spins are weak; there are as many spins up as there are down, and the total magnetization is zero. Below a critical temperature T_c , this up-down symmetry is broken, and the majority of spins point in the same direction. This phase transition is accompanied by singular behavior in the response of the system to changes in temperature; the singularities usually take the form of power laws similar to eq. (1). As an example, in Figure 1 the specific heat has been calculated exactly for a two-dimensional Ising model and displays a logarithmic dependence on $(T - T_c)$ (which can be regarded as the limiting behavior when the exponent $\alpha \rightarrow 0$).

COMPUTER SIMULATION OF THE ISING MODEL

For an Ising model with only two spins, any property can easily be calculated by summing over the four states. However, the number of states grows exponentially with the number of spins. Even for a two-dimensional 10×10 lattice, there are 2^{100} configurations to sum over, requiring more than 10^{15} years of computer time.

It might be supposed that states could be chosen at



The exact results for the $m \times n$ square lattice with periodic boundary conditions are displayed for $m = n = 2, 4, 8, 16, 32$, and 64 . The limiting critical point is marked by a vertical line. Taken from Ferdinand, A.E., and Fisher, M.E., Bounded and inhomogeneous Ising models: Specific-heat anomaly of a finite lattice, *Phys. Rev.* 185, 832 (1969).

FIGURE 1. The Specific Heat per Spin for Small Ising Lattices

random to estimate the sum. Unfortunately, the overwhelming majority of states in most systems with a large number of particles are energetically unfavorable and do not make a significant contribution. This makes random sampling so inefficient as to be completely impractical.

A better approach is to simulate the behavior of the system by generating states with the probability they would have in nature. We can easily generate a sequence of configurations for which the probability of finding each of the four states is given by eq. (4). We start with an arbitrary state and choose one of the spins using a random number generator. We then compute the change in energy required to reverse the spin (either $+2J$ or $-2J$). If the energy is lowered, the change is made for the next configuration; if the energy is raised, the change is only made with the probability $\exp(-2K)$. The choice is made by comparing $\exp(-2K)$

with another random number uniformly distributed between zero and one [8]. Any observable such as the average total energy can then be calculated by taking the mean over the configurations generated.

For a system with many particles, the situation is almost identical. Again, a sequence of configurations is generated by altering a spin according to the energy change and a comparison with a random number. The algorithm is very efficient, even for a large system, since the energy change can be computed from a small number of terms involving only the values of the nearest neighbor spins. Typical configurations for the Ising model taken from a computer simulation of a 64×64 lattice are shown at the top of Figure 2 for temperatures 10 percent above and 5 percent below the critical temperature.

The specific heat must be treated somewhat differently because it is the derivative of the energy with respect to temperature. Such derivatives can also be calculated from fluctuations within the sequence of configurations. Since the average energy is given by

$$E = J\langle S \rangle = Z^{-1} \text{Tr}_{\{s\}} JS \exp(H), \quad (9)$$

it is easy to show that

$$\frac{d\langle S \rangle}{dK} = \langle S^2 \rangle - \langle S \rangle^2, \quad (10)$$

which is essentially the specific heat, since K is the reciprocal temperature.

This method is known as Monte Carlo simulation, because of the use of random numbers as an essential feature.

LARGE CORRELATION LENGTHS AND FINITE-SIZE SCALING

Computer simulations are limited by statistical errors and the size of the systems that can be analyzed. The latter is the most serious problem in the investigation of phase transitions.

As mentioned earlier, a correlation extends over longer distances as some critical temperature T_c is approached; correlation lengths diverge at T_c . As long as correlation lengths are small in comparison with the size of the systems being simulated, the computer simulations are indistinguishable from truly macroscopic systems. Since the correlation lengths diverge at T_c , however, they are *always* larger than the model when close to T_c . Since the fluctuations over large distances are responsible for the singularities at T_c , singularities are rounded off in a finite system, as shown in Figure 1.

This can be made more quantitative by considering the effect of the finite, but large, linear dimension L of the simulated system in eqs. (1) and (2). As long as the correlation length ξ is much less than L , these equations hold. However, when ξ and L are roughly the same size, ξ stops growing, and the specific heat divergence is rounded off. This will happen for

$$\xi \approx L \propto (T - T_c)^{-\nu}, \quad (11)$$

at which point

$$C \sim (T - T_c)^{-\alpha} L^{\alpha/\nu}. \quad (12)$$

By simulating different-sized systems and plotting the height of the peak in the specific heat as a function of L , eq. (12) provides a simple method of calculating the exponent ratio α/ν . This method is known as finite-size scaling and has been used frequently to obtain information not available by analytic methods.

RENORMALIZATION GROUP ANALYSIS

The concept of examining the correlations near the critical temperature on different length scales can be extended far beyond finite-size scaling analysis to improving accuracy and efficiency by the rather elegant renormalization group approach. There are many different mathematical formulations of the renormalization group; it is essentially a way of systematically integrating out the shortest wavelength or smallest scale fluctuations to obtain information on successively longer length scales. The remaining variables form a statistical-mechanical model with the same symmetry as the original.

One illustration using the two-dimensional Ising model is replacing a local group or "block" of spins with a single spin representing the most important gross features. For example, we can take a 2×2 block and replace it by a *block spin* with the value $+1$ or -1 , according to whether most of the spins in the block are up or down (ties are decided by random number). Short-wavelength fluctuations are eliminated, but it is clear that, if most of the spins over a large area are up, then most of the corresponding block spins will be up as well. If the spins are only weakly correlated over short distances, the block-spin correlations are even weaker.

The effect of performing such a transformation directly on typical configurations generated by computer for temperatures 10 percent above and 5 percent below the critical temperature is illustrated in Figure 2. There is reduction in the number of degrees of freedom (the system becomes smaller), and the correlations in the low-temperature system become steadily stronger, until the system is in the lowest energy state (all spins up) almost everywhere. Clearly, the renormalized configurations correspond to a lower effective temperature. In the high-temperature system, correlations over 10 or more lattice constants are clearly visible in the original system but are much smaller after two transformations. Here, the effective temperature increases.

In both cases, the trend is to move further away from the critical temperature. The long-range correlations remain the same after several transformations only if the original system is at its critical temperature. This property allows the critical point to be identified with considerable accuracy from the computer simulation. The Hamiltonians describing such a sequence are then said to approach a *fixed point*.

Since the average diameter of patches of like spins is

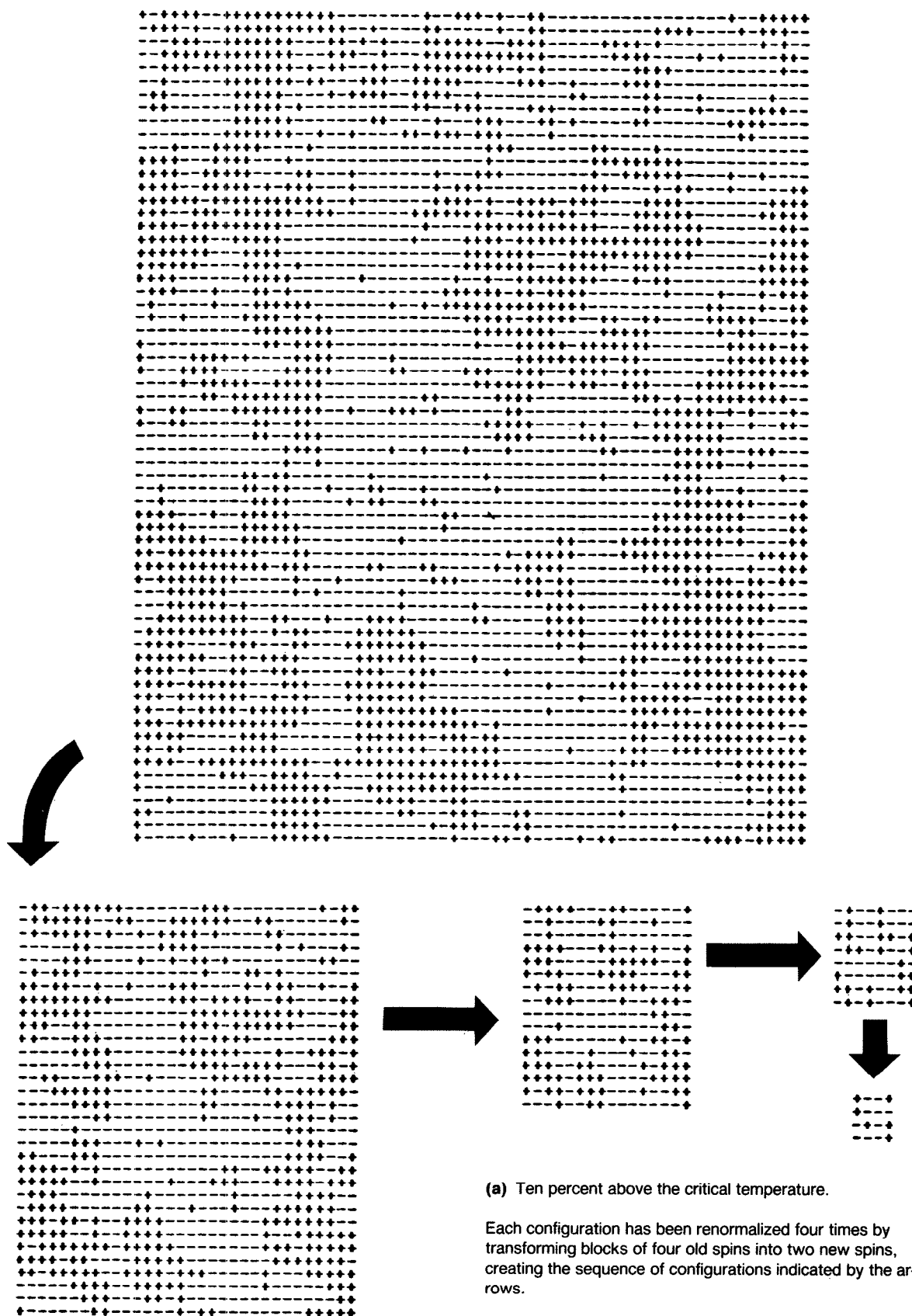
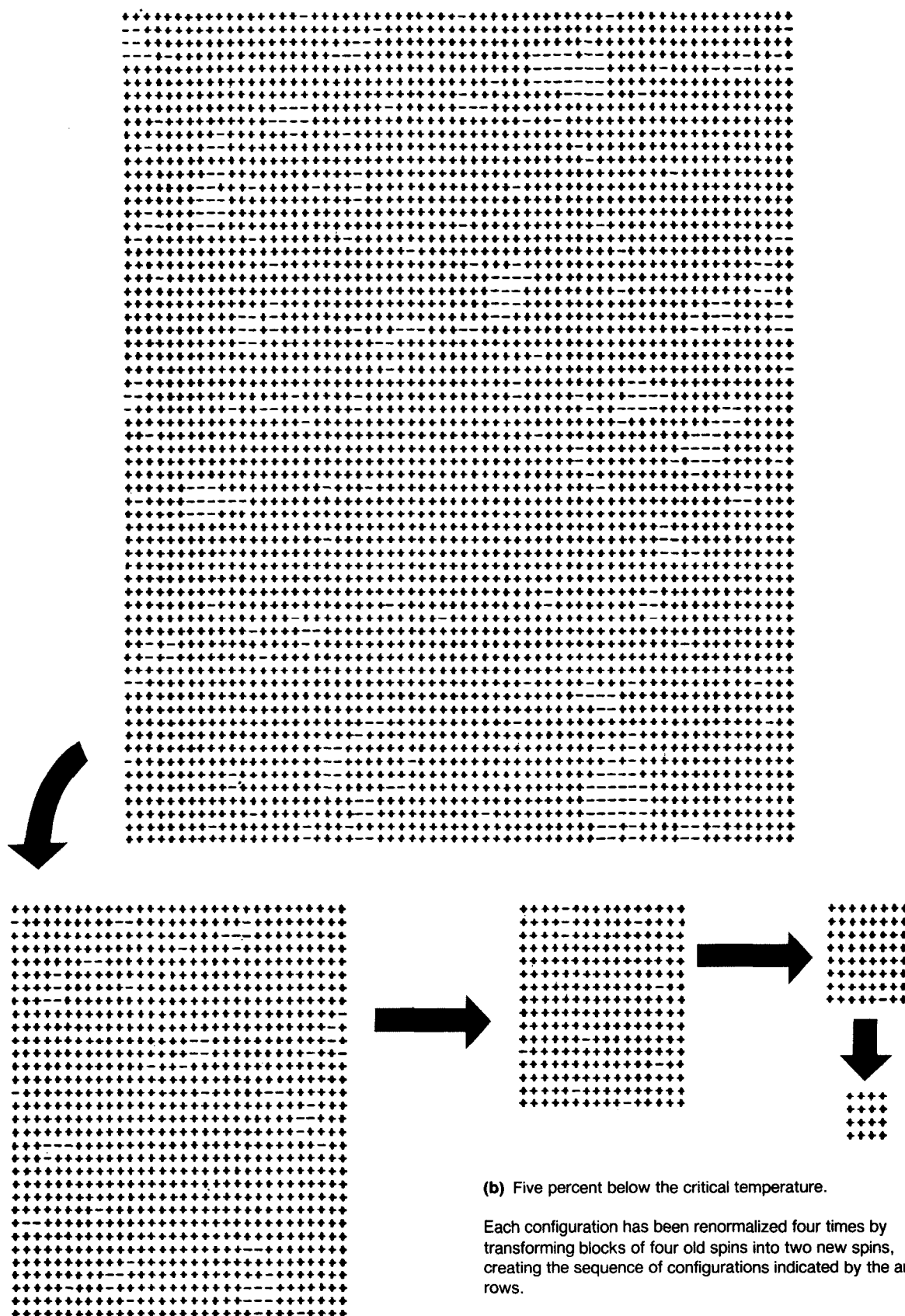
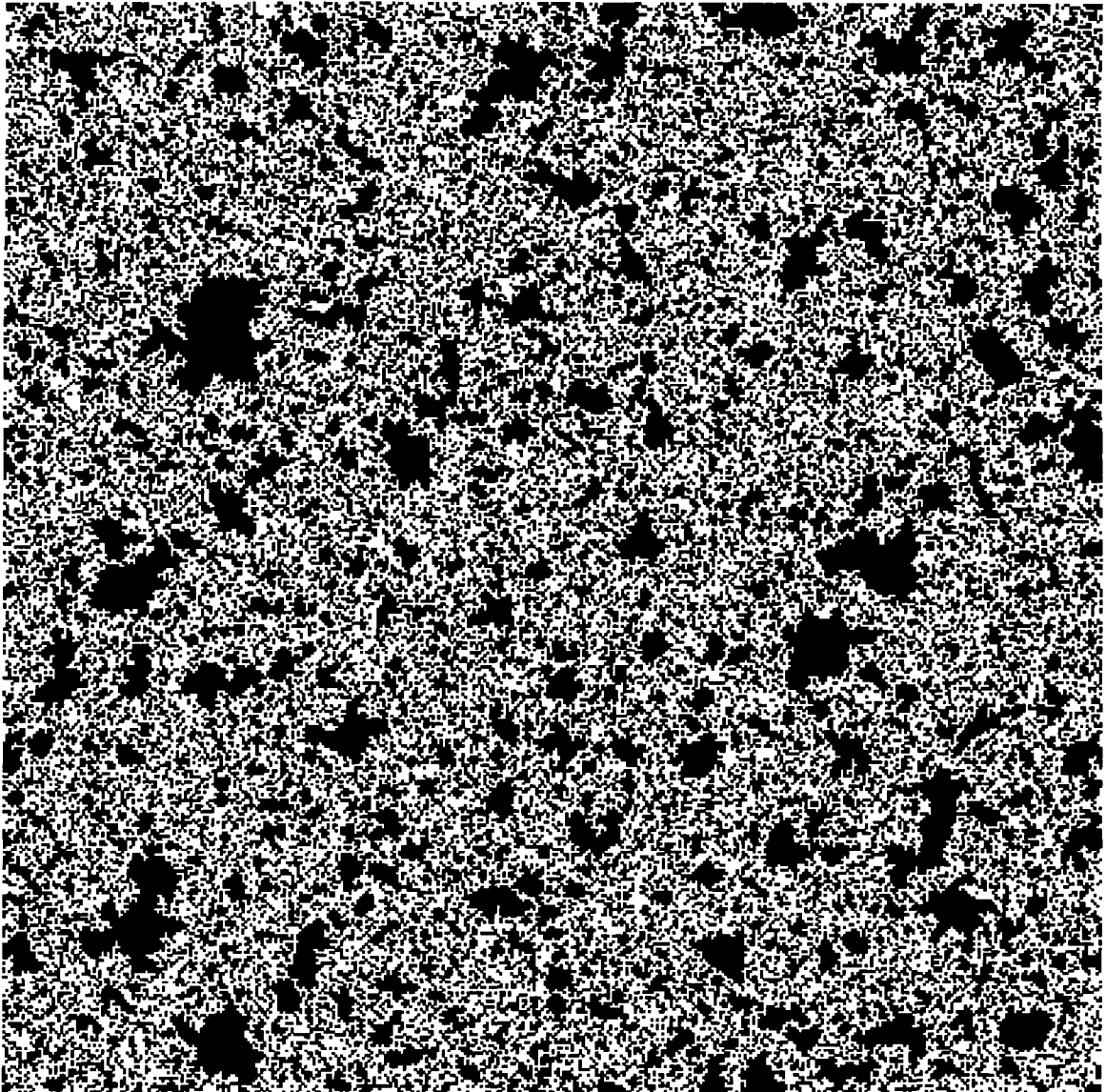


FIGURE 2a. Configurations from Monte Carlo Simulations of the $d = 2$ Ising Model

FIGURE 2b. Configurations from Monte Carlo Simulations of the $d = 2$ Ising Model



(a) For $p = 0.61$, the percolation fraction $P(p) = 0.5251$.

FIGURE 3a. Percolation Cluster (Largest Connected Component) in a Diluted Two-Dimensional 400×400 Square Array, Just above the Percolation Threshold

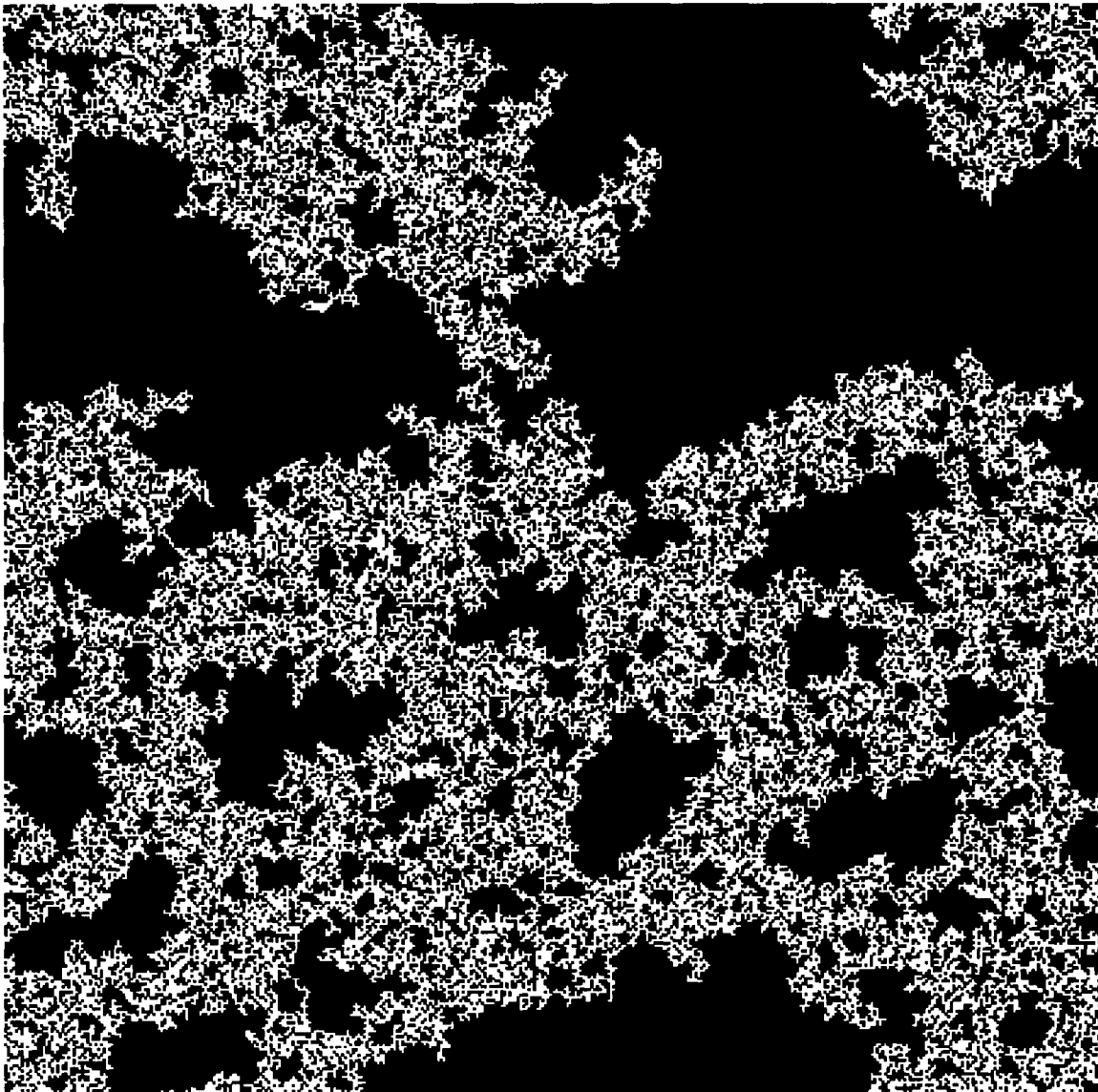
reduced by a factor of two in this example, the correlation length ξ is also divided by two. By analyzing the renormalized configurations to determine how rapidly the effective temperature moves away from the critical temperature, we can obtain a relationship between the correlation length and the effective temperature. This allows us to evaluate ν in eq. (1) and, in fact, can also be used to evaluate α and the power-law singularities for other properties of the system.

PERCOLATION PHENOMENA

The concepts developed to treat critical phenomena, especially the notions of correlation length, order pa-

rameter, scaling, and critical exponents, can be applied to situations far from the magnets or fluids usually studied in statistical mechanics. Percolation processes provide an excellent example. Consider a porous random material such as sandstone. If the pores comprise only a small fraction of the material's volume, water will not penetrate the rock. However, if the pores constitute a sufficiently large fraction of the material, water flows from pore to pore and passes through macroscopic distances of rock.

The transition between these two types of behavior with increasing porosity, $1 - p$ (the portion of the rock volume consisting of pores), is sharp, with a reproduc-



(b) For $p = 0.595$, $P(p) = 0.3260$.

FIGURE 3b. Percolation Cluster (Largest Connected Component) in a Diluted Two-Dimensional 400×400 Square Array, Just above the Percolation Threshold

ble threshold value p_c of the porosity. It is, in fact, a phase transition. This was first argued on intuitive grounds [1] and then demonstrated analytically in the context of simplified models.

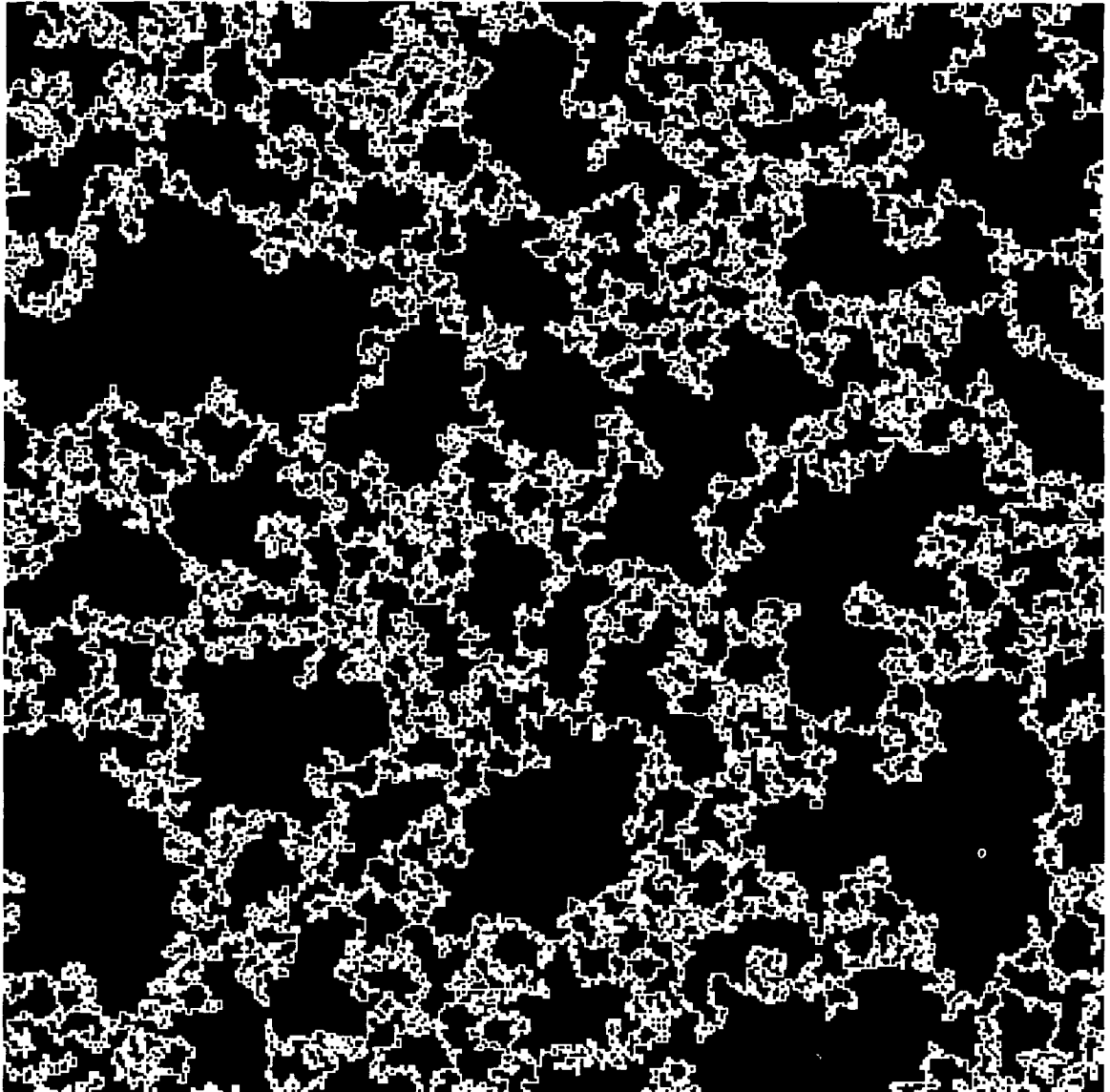
Several recent review articles have developed this connection in detail [3]. As in magnetic phase transitions, long-range phenomena (conduction of fluid) develop from short-ranged interactions (the interaction or connectedness of adjacent pores). There is a natural order parameter, usually called the percolation probability $P(p)$, which can be defined as the fraction of pores that are connected to the water-carrying portion of the rock, as the fraction of rock that is wetted by a fluid

applied at the surface of a macroscopic sample, or as the size of the largest connected cluster of pores. The three definitions have been shown to be equivalent in the limit of macroscopic sample size.

A correlation length $\xi(p)$ can also be defined for this problem by evaluating the probability that two pores, located at x and y , are connected. Below the percolation threshold, this probability will fall off exponentially with spatial separation:

$$g(x, y) \sim \exp\left(\frac{-|x - y|}{\xi(p)}\right), \quad (13)$$

while $g \rightarrow P(p)$ for $p > p_c$ and while the limit is ap-



(a) For $p = 0.61$, as in Figure 3a, the backbone fraction $B(p) = 0.2648$.

FIGURE 4a. Backbones (Largest Multiply Connected Component) for the Cluster Shown in Figure 3a

proached with an exponential decay like that in eq. (13). Similarly, the percolation probability increases above the threshold in a macroscopic sample with a critical dependence,

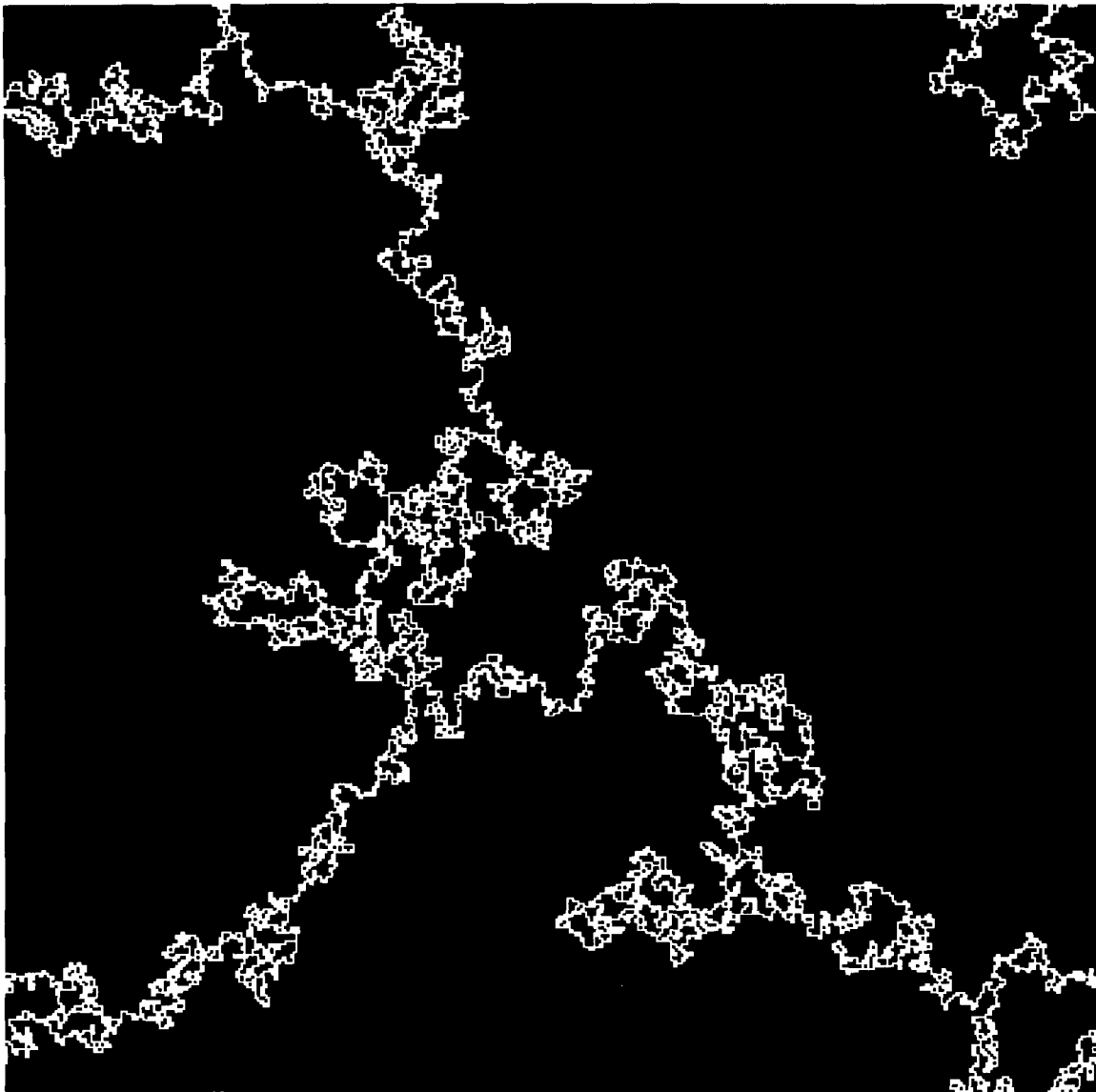
$$\begin{aligned} P(p) &\sim (p - p_c)^{\beta}, & p > p_c, \\ &= 0, & p < p_c. \end{aligned} \quad (14)$$

As in the magnetic phase transitions, continuity between the behavior of the correlation function both below and above the threshold implies that the correlation length $\xi(p)$ diverges at p_c , just as in eq. (1).

Since percolation is a geometric phenomenon, pic-

tures of the clusters obtained in the course of computer simulations can be informative. For example, Figure 3, on pages 368–369, shows in white against a black background the largest clusters found in two simulations with p close to p_c . Opposite edges of the system in Figure 3 and 4 are treated as connected. The increased correlation length as p approaches p_c in Figure 3b should be apparent from the increasing size of the missing regions. In this figure, $\xi(p)$ is comparable to the size of the region shown.

As is the case in conventional phase transitions, finite-size scaling can be used to analyze simulations of



(b) For $p = 0.595$, as in Figure 3b, $B(p) = 0.0765$.

FIGURE 4b. Backbones (Largest Multiply Connected Component) for the Cluster Shown in Figure 3b

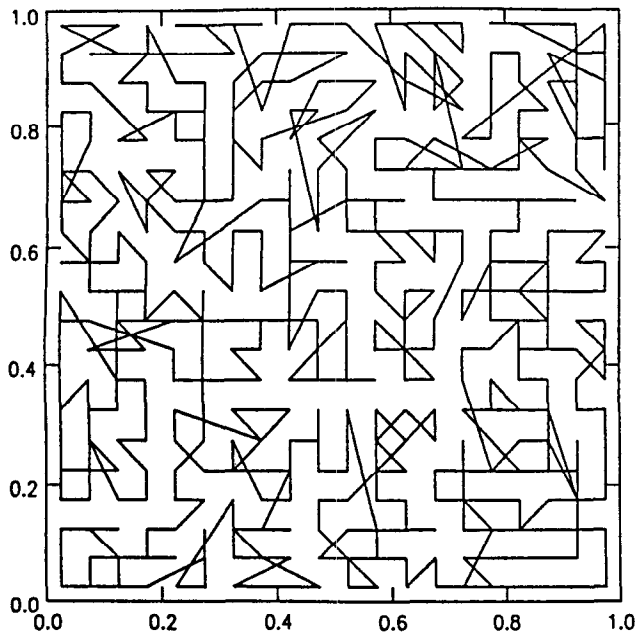
percolation. For example, if $p \sim p_c$, so that the coherence length $\xi(p)$ exceeds the linear dimension of the model L , we find

$$P(p, L) \sim L^{-\beta/\nu}. \quad (15)$$

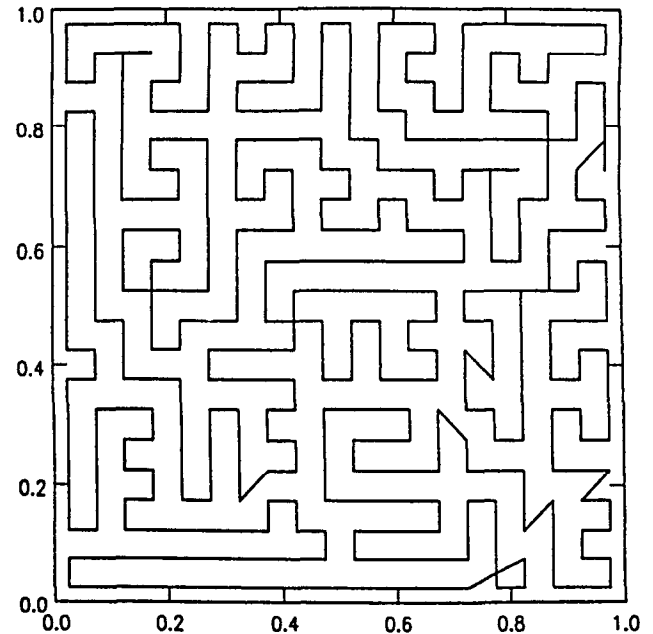
The largest connected component in this limit is a fractal object [7], since its volume $P(p, L)L^d$ has an anomalous dependence on its linear dimension L . The exponent $d - \beta/\nu$ is a fractal dimensionality characterizing the space in which percolation flow first occurs.

Standard graph-theoretical algorithms are useful for analyzing the statistics of clusters generated in percola-

tion simulations. For example, actual fluid flow through a region of interconnected pores will only occur in volumes across which a pressure differential can develop. If a volume can be disconnected from the bulk by plugging a single pore, then it will not support flow. All such "tag ends" can be disconnected from the percolating region, represented as a large graph, by using standard backtracking methods for obtaining doubly connected components of undirected graphs [1]. The result of this analysis is shown in Figure 4, which depicts the largest multiply connected components, or "backbones," of the clusters shown in Figure 3. Further



(a) For 400 points, temperature $T = 1.0$ and the mean length per step $l = 1.85$.



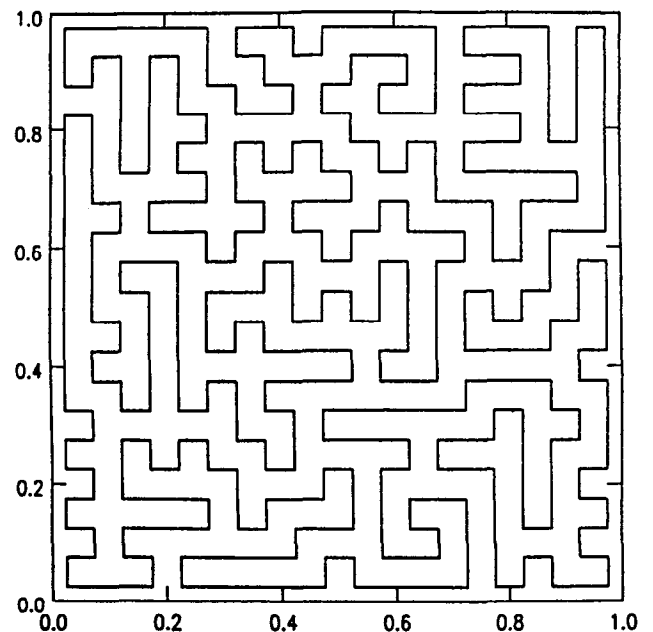
(b) 400 pts., $T = 0.3$ and $l = 1.04$.

analysis can give information on the shortest paths that cross the infinite cluster at threshold, or the number of parallel paths. These characteristics also show critical behavior at p_c and can be related to experimental properties of composites that are comprised of superconducting and normal metallic grains.

SPIN GLASSES

Much recent work has been done on the effects of disorder on conventional phase transitions, such as the transitions from gas to liquid to solid, or from a paramagnet (with atomic spins disordered) to a ferromagnet (with atomic spins aligned). The simplest sort of disorder to model is dilution; in magnetic systems this can occur when magnetic atoms are diluted with nonmagnetic atoms. For small amounts of dilution, the effect is a quantitative change in, for example, the temperature at which ordering occurs. For greater degrees of dilution, percolation effects can be observed. The magnetic atoms become separated into finite clusters of interacting atoms, isolated from one another, and the ordering temperature is reduced, tending continuously to zero at the percolation concentration.

When the randomness in the system introduces conflict between incompatible types of interactions, new physical phenomena are observed. In some magnetic alloys, the fact that the separation between magnetic atoms varies over a wide range not only weakens some of the interactions but causes some of the interactions to be ferromagnetic in sign, favoring parallel alignment of the atomic spins, whereas other interactions are antiferromagnetic, or opposite in sign. There is no general way that the spins can be made to satisfy all the interactions they are subject to in this situation, so such



(c) 400 pts., $T = 0$ and $l = 1$.

FIGURE 5. Solution of a Traveling-Salesman Problem by Simulated Thermal Annealing

systems are termed "frustrated" [9]. Such disordered systems are highly degenerate and disordered at low temperatures.

Magnetic systems of this type are termed *spin glasses*

because of the analogy between their magnetic state at low temperatures and the amorphous structures that result in quenching from the melt substances that are too disordered or viscous to crystallize. In principle, these degenerate pseudoground states are metastable, although it is possible to observe, when the temperature is low enough, that the relaxation times associated with the decay of one such state into another become astronomically long. A spin glass is thus magnetically rigid, just as window glass is structurally rigid.

Constructing and analyzing such glassy low-energy states are optimization problems having much in common with traditional optimization problems in applied mathematics and engineering. Exact determination of the ground state of a model can be shown to be an NP-Complete problem in some simple cases, which means that heuristics are needed to study model systems with thousands of spins. Early efforts relied on iterative improvement procedures of an obvious sort; eventually it became clear that the most efficient way to search for the low-energy states of a spin glass was to use Metropolis simulation to mimic the physical process of slow cooling through the temperature at which the spins freeze, and careful annealing in the ordered phase [5].

OPTIMIZATION

This observation about spin glasses can be of use in optimizing engineering problems [4]: The frustration that introduces degeneracy and metastability into spin glasses is also a common feature of hard optimization problems for which a solution subject to conflicting constraints must be found. For example, in assigning places to thousands of circuits in a computer, we must place the circuits close together so that the wires needed to connect them will be as short as possible. We must also leave enough room between the circuits for the package to be able to accommodate the wire required without overflowing. This problem clearly exhibits frustration, but the analogy to spin glasses implies that there must be many acceptable solutions to the problem if there are any. It should therefore not be necessary to find the absolute optimal solution.

A more easily formalized optimization problem is the well-known *traveling-salesman* problem, which requires us to construct the shortest tour of a prescribed list of N cities. The frustration arises between keeping the path short and requiring it to be a tour. An example of the application of simulated annealing to a traveling-salesman problem is shown in Figure 5.

For the problem to have a known solution, the cities in this example have been put on the points of a regular 20×20 square grid. The optimal path can be no shorter than one grid spacing per step, and it is possible to convince oneself that such a tour is possible. To rearrange the salesman's path, it suffices to select an arbitrary subsequence of points in the existing path and then to reverse the order in which they are traversed. This basic move is the simplest of a set introduced to the problem by Lin and Kernighan [6]. With the extra

power of annealing, this is sufficient to obtain solutions, for problems with a few thousand cities, that are as good as the solutions found with more time-consuming exhaustive searches employing more elaborate moves.

At high temperatures (Figure 5a), the salesman's path follows the underlying grid for only a few steps at a time. At lower temperatures, the path is optimal for very long distances, with mistakes occurring in isolated local regions (Figure 5b). Such mistakes cannot be removed by the basic subsequence reordering move, but they do diffuse about until two defects meet and annihilate each other. Finally, the process concludes with one of the many possible exact minimum-length tours (Figure 5c).

The sequence of phenomena occurring from a high to a low temperature is quite like that occurring as liquids solidify, with a slowly growing distance of ordering at the high temperature, and the excess energy at the low temperatures associated with locally stable defects that can only be removed by diffusion to the surface or recombination. Experience with several optimization problems and the simulated annealing process for attacking them [4] suggests that the metaphor connecting statistical physics in disordered matter and the sorts of hard optimization problems that arise in the engineering of complex systems is a profound one, capable of providing useful insights for the devising of effective heuristics.

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