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Monte Carlo Simulation of Three-Dimensional Dilute Ising Model

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A multispin coding program for site-diluted Ising models on large simple cubic lattices is described in detail. The spontaneous magnetization is computed as a function of temperature, and the critical temperature as a function of concentration is found to agree well with the data of Marro et al.[4] and Landau[3] for smaller systems.

KEY WORDS: Dilute Ising model, percolation threshold, critical exponents, relaxation time.

1. INTRODUCTION

In the randomly dilute quenched Ising model investigated here each site on a simple cubic lattice is randomly either occupied, with probability p, by a spin $\frac{1}{2}$ atom, or by a nonmagnetic atom. The spins interact via nearest-neighbor exchange energies J. The Curie temperature $T_c(p)$ decreases with decreasing p and reaches zero at the percolation threshold p_c (Ref. 1).[3] For equilibrium properties one would like to know what the critical exponents would be if $T_c(p)$ is approached at fixed p. Theoretically[1,2] one expects $0 < p < p_c$ exponents independent of p but different from those for $p = 1$. However, older simulations[3] up to system size 30^3 found no change in these exponents compared to $p = 1$, and recent work[4] with system size 40^3 found them to change continuously with p. Thus we try to find out, by

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[3] The first successful epsilon expansion seems to be by D. E. Khmelnitskii, *ZhETF* **68**:1960 (1975), English translation *Sov. Phys. JETP* **41**:981 (1975); for numerical estimates see K. E. Newman and E. K. Riedel, *Phys. Rev.* **H25**:264 (1982), for experiments see R. J. Birgenau, R. A. Cowley, G. Shirane and H. Yoshizawa, *J. Stat. Phys.* **34**:817 (1984).

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simulating systems with 90^3 spins, if these latter results again are due to the finite system size.

For dynamic aspects one would like to know[5–11] how the relaxation time diverges at the percolation threshold and how the magnetization decays to zero there if one starts the simulation with all spins parallel. We study this relaxation time,[5] along the line $\exp(-2J/kT) = 1 - p/p_c$ in the T–p diagram, which is more convenient for Monte Carlo simulation than the lines $T=0$ or $p=p_c$. Traditional scaling theory[1] expects the same exponents along any straight line in the $\exp(-2J/kT)$ versus p diagram which approaches the percolation point $T=0$, $p=p_c$ with a slope not tangent to the phase transition line.[12] Again a system size 90^3 is used and we work with the nonlinear relaxation time.[13]

The main part of this paper consists of an explanation of how to program dilute Ising models with multi-spin coding (Section 2) whereas our results are summarized in Section 3.

2. COMPUTATIONAL DETAILS

MC simulation of large cubic dilute Ising modes (90^3) were carried out on a Cyber CDC 176 scalar computer. In order to accommodate the 90^3 lattice sites within the memory of this computer we used multispin coding. In this technique one stores many spins in one single computer word consisting of 60 bits and performs logical bit–bit operations with them. The most common among these logical operations are logical OR, logical AND, exclusive or XOR, and SHIFT (see Ref. 14 for an introduction). Pure Ising model systems as large as 1080^3 had been simulated earlier by this method[15] and complete computer programs used for these simulations have been published.[16,17] We have modified the latter program so as to adopt it for dilution. The basic idea is very similar to that adopted[18] for the simulation of the Random-Field Ising Model (RFIM). In the latter problem one has to store not only the spin orientation at every lattice site but also the orientation of the (random) magnetic field at that site. In the case of pure Ising model on simple cubic lattice with no random field, one stores each spin in three bits (in fact, every third bit from the left is either 1 or 0 depending on the corresponding spin being "up" or "down"), and thus 20 spins can be stored in a 60-bit computer word. In the case of the RFIM, every fourth bit from the left was used to store the orientation of the (random) magnetic field at the spin which was being stored in the preceeding three bits (see Ref. 18). Therefore, in that case, 15 spins could be stored in a 60-bit computer word.

In the dilute Ising model (there is no random external field as in RFIM) we have used every fourth bit from the left to store the occupation

number of the corresponding lattice site; occupation number 1 corresponds to the site being occupied by a spin, otherwise the occupation number is set equal to zero. For economy of words, the sites occupied by the magnetic atom (spins) will be called "occupied"; sites containing no spin will be referred to as "empty." Suppose p is the concentration of the occupied sites. The spatial configuration (i.e., the configuration of the randomly "occupied" sites), was initialized by the FORTRAN statement

$$\text{ICI} = \text{ICI.OR.(IFIX(1 + p - RANF(0)))}$$

followed by a circular left shift of ICI by four bits. At the beginning ICI was 0 and at the end of its initialization the spin word IS(I, J, K) was set equal to ICI, for $K = 1, 2, \ldots, L$, $J = 1, 2, \ldots, L$ and $I = 1, 2, \ldots, LL = L/15$. This kind of initialization of the random occupation of the sites also produces the initial orientation of the spins—all the spins point "down" (every third bit of the 4-bit parcels being zero), no matter whether the corresponding lattice site is occupied or empty! In other words, we have "ghost spins" at the empty sites. However, in our subsequent computation we never compute the number of down-spin neighbors of any arbitrary site directly from the number of zeroes at the third bits, but we shall infer it indirectly from the difference between the number of occupied sites and the number of up-spin neighbors. Moreover, the "ghost spins" at the empty sites will never be flipped during the simulation.

As stated earlier, the occupation status and the spin orientation at an arbitrary lattice site are stored at the third and the fourth bits, respectively, of each of the 4-bit parcels. In order to read the content of the fourth bit ignoring the contents of the first three bits, we define a mask IEN1 consisting of the bit string 000100010001.... (15 repetitions of the 4-bit sequence 0001). Now, with ICI as the abbreviation for IS(I, J, K),

$$\text{IOCC} = \text{ICI.AND.IEN1}$$

contains only the desired information on the occupation number of the 15 sites stored in the corresponding computer word. Similarly, in order to read the contents of the first three bits, ignoring the fourth one in each of the 4-bit parcels, we define another mask IEN14 consisting of the bit string 111011101110.... (15 repetitions of the 4-bit sequence 1110). Now, the desired information is contained in the last three bits of the 4-bit parcels of

$$\text{ISPIN} = \text{SHIFT((ICI.AND.IEN14),59)}$$

Next we have to compute the energy of interaction $JS_i\Sigma S_j$ between each spin S_i and its occupied nearest neighbors. (In this discussion we set $J = 1$ and $k_B = 1$.) Then we compute the change in energy ΔE that would take place if the spin at the ith site is flipped. In the usual representation of Ising

spins by 1 and -1 the sum ΣS_j on a simple cubic lattice without dilution can have the even integer values between -6 and $+6$, i.e., $\Sigma S_j = -6$, -4,..., 4, 6 and, consequently, the corresponding $\Delta E = 12$, 8,..., 8, -12 if the central spin S_i is up. An effect of dilution is that now odd-integer values of ΣS_j are also allowed, i.e., $\Sigma S_j = -6$, -5,..., 5, 6. Therefore, now all the even integers between 12 and -12 are allowed values of ΔE.

Second, in our simulation we have used the (0, 1) representation of the Ising spins where 1 stands for up and 0 stands for down. Therefore, proper care has to be taken in computing ΔE. We first compute two quantities IOCCT and ISPINT (see Table I). Each of the 4-bit parcels of IOCCT gives the total number of occupied nearest-neighbor sites of the spin stored in the corresponding four bits of IS(I, J, K). Similarly, each of the 4-bit parcels of ISPINT gives the total number of up-spin nearest-neighbors of the spin stored in the corresponding four bits of IS(I, J, K). Then each of the 4-bit parcels of (IOCCT-ISPINT) gives the total number of down-spin nearest-neighbors of the spin stored in the corresponding four bits of IS(I, J, K), and each of the 4-bit parcels of ISPINT–(IOCCT-ISPINT) gives the difference between the number of up-spin and down-spin neighbors of the spin stored in the corresponding four bits of IS(I, J, K). Now IEN7 consists of the bit string 01110111... (15 repetitions of the 4-bit sequence 0111). Thus, the numbers stored in each of the 4-bit parcels of the quantity

$$\text{IN} = \text{IEN7} + \text{ISPINT} - (\text{IOCCT-ISPINT})$$

can vary between 1 and 13. However, we have to take the spin of the central site (I, J, K) into account in order to compute the interaction energy. ISP15 has 1111 in the 4-bits if the corresponding bits in IS(I, J, K) correspond to an up spin and has 000 otherwise. Thus, the numbers stored in each of the 4-bit parcels of IN + ISPIN can vary between 1 and 14. Each of the 4-bit parcels of $A = \text{XOR}(\text{IN} + \text{ISPIN}, \text{ISP15})$ contains the information about the change in energy ΔE, namely, that $2(A-7)$ is the expected energy change if the spin in IS(I, J, K) which corresponds to that 4-bit parcel is flipped. Now, as in the case of the pure Ising model,[17] one has to investigate separately for each spin whether or not the spin under consideration has to be flipped. This requires comparison of the corresponding Boltzmann number with a random number, as in usual Metropolis algorithms. We read the contents of the last (rightmost) four bits of $\text{IN} = \text{XOR}(\text{IN} + \text{ISPIN}, \text{ISP15})$ by a logical AND with the number ...00001111(=15) and then collect the corresponding flip probability $\exp(2 * (\text{IN} - 7)/T)$ under this index in our table of the Boltzmann factors. (The Boltzmann factors $\exp(2 * (I-7)/T)$ for $I = 1$, 13 were stored once for all for a given T in the beginning of the computation.) The random num-

Table I. Main Part of the FORTRAN Program

```
      DO 251 K = 1, L
      DO 251 J = 1, L
      DO 251 I = 1, LL
      ICI = 0
      DO 250 II = 1, 15
      ICI = ICI.OR.(IFIX(1 + P - RANF(II)))
C     IF(RANF(II).LT.P)ICI = ICI.OR.1
250   ICI = SHIFT(ICI, 4)
251   IS(I, J, K) = ICI
      DO 7 ITIME = 1, ITIMX
      DO 4 K = 1, L
      KP1 = INDP1(K)
      KM1 = INDM1(K)
      DO 4 J = 1, L
      JP1 = INDP1(J)
      JM1 = INDM1(J)
      DO 4 I = 1, LL
      ICI = IS(I, J, K)
      IF(I.EQ.1)GO TO 10
      IF(I.EQ.LL)GO TO 11
      IOCCT = (IS(I - 1, J, K).AND.IEN1) + (IS(I + 1, J, K).AND.IEN1)
      ISPINT = (SHIFT((IS(I - 1, J, K).AND.IEN14), 59)) +
     &         (SHIFT((IS(I + 1, J, K).AND.IEN14), 59))
      GO TO 12
10    IOCCT = (IS(2, J, K).AND.IEN1) + ((SHIFT(IS(LL, J, K), 56)).AND.IEN1)
      ISPINT = (SHIFT((IS(2, J, K).AND.IEN14), 59)) +
     &         (SHIFT(((SHIFT(IS(LL, J, K), 56)).AND.IEN14), 59))
      GO TO 12
11    LLM1 = LL - 1
      IOCCT = (IS(LLM1, J, K).AND.IEN1) + ((SHIFT(IS(1, J, K), 4)).AND.IEN1)
      ISPINT = (SHIFT((IS(LLM1, J, K).AND.IEN14), 59)) +
     &         (SHIFT(((SHIFT(IS(1, J, K), 4)).AND.IEN14), 59))
12    IOCCT = IOCCT + (IS(I, JM1, K).AND.IEN1) + (IS(I, JP1, K).AND.IEN1)
     &              + (IS(I, J, KM1).AND.IEN1) + (IS(I, J, KP1).AND.IEN1)
      ISPINT = ISPINT + (SHIFT((IS(I, JM1, K).AND.IEN14), 59))
     &                + (SHIFT((IS(I, JP1, K).AND.IEN14), 59))
     &                + (SHIFT((IS(I, J, KM1).AND.IEN14), 59))
     &                + (SHIFT((IS(I, J, KP1).AND.IEN14), 59))
      IN = IEN7 + ISPINT - (IOCCT-ISPINT)
      ISPIN = SHIFT((ICI.AND.IEN14), 59)
      ISP15 = ISPIN.OR.SHIFT(ISPIN, 1).OR.SHIFT(ISPIN, 2)
     & .OR.SHIFT(ISPIN, 3)
      IN = XOR(IN + ISPIN, ISP15)
      ICH = 0
      DO 3 II = 1, 15
      IN = SHIFT(IN, 4)
      ICH = SHIFT(ICH, 4)
      ICDC = ICDC * MULT
      ID1 = ICDC - IEX(IN.AND.15)
      IF(LD1)ICH = ICH.OR.2
3     CONTINUE
      ICH = ICH.AND.SHIFT ICI.AND.IEN1, 1)
      IS(I, J, K) = XOR(ICI, ICH)
4     CONTINUE
      M = 0
      DO 54 K = 1, L
      DO 54 J = 1, L
      DO 54 I = 1, LL
54    M = M + COUNT(IS(I, J, K).AND.IEN2)
```

bers, required for comparison, were generated, following Kalle, as random integers between 1 and 2 ** 48 by a simple multiplication of a number by a suitable multiplier. Then the subtraction of the Boltzmann factor IEX, properly normalized by a factor 2 ** 48, from ICDC yields a 0 or 1 in the last (rightmost) bit of the computer word

$$\text{ID1} = \text{ICDC} - \text{IEX(IN.AND.15)}$$

depending on whether ICDC is larger or smaller than IEX. Next we initialized a changer word ICH to be 0 (all the bits are set to 0). With the help of a logical variable LD1 (LD1 is equivalenced to ID1 in the beginning of the program), we change the third bit of the corresponding 4-bit parcel in the changer word ICH to a 1 (logical *OR* with number 2) if the spin has to be flipped; otherwise we keep the zero there. However, we must take into account the fact that the "ghost spins" at the empty site must not be flipped. In order to implement that scheme, we compute

$$\text{ICH} = \text{ICH.AND.SHIFT(ICI.AND.IEN1, 1)}$$

If a lattice site is occupied, the corresponding four bits in ICH remain unaltered by this operation. On the other hand, if a lattice site is empty, the corresponding four bits in ICH are set equal to zero by this operation. Finally, XOR(ICI, ICH) flips or does not flip the individual spins depending on whether there is a 1 or 0 at the third bit of the corresponding 4-bit parcel in ICH.

3. RESULTS

The longest Monte-Carlo time up to which we continued the simulation for a given p and T is 8000 MCS. The $T_c(p)$ values thus determined are shown in Table I. The effective exponents were determined from the equilibrium magnetization data for reduced temperatures $(T_c - T)/T_c$ varying between 0.03 and 0.1. The effective exponent β thus computed was found to increase continuously with the dilution ($\beta = 0.29$, 0.28, 0.31, and 0.37 for $p = 1.00$, 0.95, 0.90, and 0.80, with error bars near ± 0.02). Thus, while Marro et al.[4] found results differing from those of Landau[3] by using larger systems ($L = 40$ instead of L up to 30), we went to even larger systems ($L = 90$) and confirmed the trend observed by Marro et al. However, we believe that this trend is a consequence of the fact that in order to observe true critical behavior one needs to compute the equilibrium magnetization much closer to the critical point. With our data we are unable to distinguish reliably between a continuous variation of the true exponent β with p, and the theoretically expected p-independent β combined with a p-dependent amplitude for a correction-to-scaling term.

Table II. Concentration Dependence of the Critical Temperature

p	$T_c(p)/T_c(1)$
1.0	1.0 ± 0.0013
0.95	0.9451 ± 0.0013
0.90	0.8935 ± 0.0013
0.80	0.7771 ± 0.0013
0.70	0.6750 ± 0.0013
0.60	0.5563 ± 0.0013
0.50	0.4363 ± 0.0013
0.40	0.3212 ± 0.0025
0.35	0.2475 ± 0.0025

Such an analysis could not be achieved with this general-purpose computer and remains a challenge for special-purpose machines.

For the nonlinear[13] relaxation time $\tau = \int M(t)\,dt$ we have already reported our results.[5] (We start with all spins up and then let them flip with probability $1/(1+\exp(\Delta E/kT)$ where ΔE is the energy change connected with that change.) Mainly we found that a normal power law, $\log \tau \propto \log(p_c - p) + \cdots$, does not fit the data well, whereas a parabolic fit,[6,7,10] $\log \tau \propto \log^2(p_c - p) + \text{const.}\ \log(p_c - p) + \cdots$, or an exponential variation, like $\log \tau \propto 1/(p_c - p)^{1/2}$, work nicely. The data are also consistent with a power divergence at a shifted critical point near $p = 0.30$. The decay of $M(t)$ from about unity to about zero is roughly logarithmic in time, whereas a power law in t fits badly. Additional simulations at $p = p_c$ for various temperatures were qualitatively consistent with our more accurate data along the line $\exp(-2J/kT) = 1 - p/p_c$.

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NOTE ADDED IN PROOF

For the square lattice, S. Jain (*J. Phys. A* **19**, Letters), gives further Monte Carlo results on correlation function and relaxation; and B. Derrida *et al* employ the "exact" transfer matrix technique to check for universal behavior.

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