strains to occur for As-doped Si, even at high doping levels. Therefore, we conclude that the large effects observed for As-doped samples are due to the presence of the d electrons in As. The As impurities will introduce either true localized levels or resonance states lying well below the top of the valence band ($\Gamma_{25'}$) at the Brillouin-zone center. Orthogonality and screening effects due to the d electrons may influence the *energy levels* of higher-lying states (in both the valence and conduction bands) but it will probably not alter greatly the joint density of states. It is much more likely that the presence of the d orbitals produces a rapid increase in many matrix elements of the dipole operator which vanish in the perfect crystal; the inclusion of d orbitals in the basis set introduces the possibility that strong $p \rightarrow d$ transitions can occur *on the same atom* where $\langle p|r|d\rangle$ is expected to be large. Thus, although the coefficient of the d orbitals may be rather small, the strength of the matrix elements and the fact that there are ten d electrons will lead to a rapid increase in α as the concentration of As increases. In B- and P-doped Si the enhancement of α will not be nearly so great because the outer s and p orbitals of B and P do not differ significantly from their counterparts in the host Si lattice.

This research was sponsored by the Division of Materials Sciences, U. S. Department of Energy, under Contract No. W-7405-ENG-26 with Union Carbide Corporation.

[1]W. C. Dash and R. Newman, Phys. Rev. 99, 1151 (1955).

[2]H. R. Philipp and E. A. Taft, Phys. Rev. 120, 37 (1960).

[3]A. A. Vol'fson and V. K. Subashiev, Fiz. Tekh. Poluprovodn. 1, 397 (1967) [Sov. Phys. Semicond. 1, 327 (1967)].

[4]M. Balkanski, A. Aziza, and E. Amzallag, Phys. Status Solidi 31, 323 (1969).

[5]H. Engstrom, J. Appl. Phys. 51, 5245 (1980).

[6]See, for example, D. Redfield, Appl. Phys. Lett. 33, 531 (1978); R. W. Keyes, Comments Solid State Phys. 7, 149 (1976); G. D. Mahan, J. Appl. Phys. 51, 2634 (1980).

[7]D. E. Aspnes, G. K. Celler, J. M. Poate, G. A. Rozgonyi, and T. T. Sheng, J. Electrochem. Soc. 80–81, 414 (1980).

[8]C. W. White, S. R. Wilson, B. R. Appleton, and F. W. Young, Jr., J. Appl. Phys. 51, 738 (1980).

[9]R. T. Young, C. W. White, G. J. Clark, J. Narayan, W. H. Christie, M. Murakami, P. W. King, and S. D. Kramer, Appl. Phys. Lett. 32, 139 (1978).

[10]C. W. White, P. P. Pronko, S. R. Wilson, B. R. Appleton, J. Narayan, and R. T. Young, J. Appl. Phys. 50, 3261 (1979).

[11]D. M. Zehner, C. W. White, G. W. Ownby, and W. H. Christie, in *Laser and Electron Beam Processing of Materials*, edited by C. W. White and P. S. Peercy (Academic, New York, 1980), p. 201.

[12]S. N. Jasperson and S. E. Schnatterly, Rev. Sci. Instrum. 40, 796 (1969).

Dynamic Monte Carlo Renormalization Group

Jan Tobochnik
Department of Mathematics, Rutgers University, New Brunswick, New Jersey 08903

and

Sanjoy Sarker and Robert Cordery
Serin Physics Laboratory, Rutgers University, Piscataway, New Jersey 08854

(Received 14 November 1980)

A novel dynamic Monte Carlo renormalization-group method is devised. Application to the kinetic Ising model in one dimension yields a value of z, the dynamic critical exponent, which is in excellent agreement with the exact result. In two dimensions we find $z = 2.22 \pm 0.13$ with the most probable value $z = 2.17$.

PACS numbers: 75.10.Hk, 75.40.Dy, 05.50.+q

Recently the Monte Carlo and renormalization-group methods have been combined to analyze a number of problems in critical phenomena.[1-4] In this Letter we extend the procedure used in Refs. 3 and 4 to dynamic critical behavior and apply our method to the computation of the dynamic expo-

nent, z, for the one- and two-dimensional kinetic Ising model.

We first review the static method. A more detailed discussion is given in Ref. 4. We describe the method for the Ising model, although it can be easily generalized to other models. The reduced Hamiltonian is defined as

$$\mathcal{H}(T) = T^{-1} \sum_{\langle ij \rangle} S_i S_j, \quad S_i = \pm 1, \tag{1}$$

where $\langle ij \rangle$ are nearest-neighbor sites on a d-dimensional hypercubic lattice, and T is the dimensionless temperature.

The first ingredient of the method is a sequence of spin configurations generated on a large finite lattice with periodic boundary condition by the traditional Monte Carlo procedure of Metropolis.[5] Block-spin configurations are constructed from the spin configurations by means of the majority rule.[6] Ties are broken by randomly assigning the block spins the value ± 1. Configurations with larger-sized block spins are constructed from those with smaller-sized block spins. If b is the size of the first block spin in units of the original lattice spacing then all lengths in the block-spin system in units of the block-spin lattice spacing have been reduced by a factor b. This leads to a reduction in the correlation length, ξ, of the infinite system by a factor b. The goal of our procedure is to find two temperatures, T_1 and T_2, such that $\xi(T_1) = b\xi(T_2)$. To do this we wish to find a renormalized Hamiltonian derived from $\mathcal{H}(T_2)$ after m iterations of the renormalization group which equals that derived from $\mathcal{H}(T_1)$ after $m+1$ iterations. If two Hamiltonians are equal then any thermodynamic average based on those Hamiltonians are equal and also further iterations of the renormalization group will continue to give equal Hamiltonians.

To be more concrete we compute the following thermodynamic averages from our Monte Carlo–generated spin and block-spin configurations:

$$E(N, m, T) \equiv (N^{(m)})^{-1} \langle \sum_{\langle ij \rangle} S_i^{(m)} \cdot S_j^{(m)} \rangle_{T,N}, \tag{2}$$

where N is the number of spins in the original lattice, $N^{(m)}$ is the number of block spins $S^{(m)}$, generated by m blockings. Only nearest-neighbor block spins are used in the above average. T is the temperature of the original spin system. We used these quantities to determine if two renormalized Hamiltonians are the same, that is, we search for two temperatures T_1 and T_2 such that

$$E(N, m, T_2) = E(Nb^d, m+1, T_1), \tag{3}$$

for m greater than some value. d is the dimensionality of the lattice. It is necessary to use a larger spin lattice for the larger block spins since we must compare block-spin averages from lattices with the same number of block spins. The above equality will only begin to occur for m sufficiently large that the effects of irrelevant interactions is small. It is essential that the matching occurs for more than one value of m to ensure that the renormalized Hamiltonians derived from T_1 are tracking those derived from T_2 and are thus equal. If matching occurs when $T_1 = T_2$, then $\xi(T_1) = b\xi(T_1)$ and T_1 must be the critical temperature T_c.

In addition the exponent ν can be computed from the equation

$$\xi(T_1)/\xi(T_2) = b = [(T_2 - T_c)/(T_1 - T_c)]^{\nu}. \tag{4}$$

In a rough calculation at T_1, about 1% above T_c, we found $\nu = 1.07 \pm 0.15$ for the two-dimensional (2D) Ising model. In this calculation, as well as the dynamic calculations, we used about one million passes on a 256-spin lattice to generate averages, which we matched to those generated from four million passes on a 64-spin lattice. A pass consists of N attempted spin flips where the spins are chosen randomly. At T_c, spins are flipped on approximately 20% of the attempts. We found matching for $m = 1$ and $m = 2$ but not for $m = 0$, with $b = 2$. Since matching occurs for small values of m, the effect of irrelevant interactions dies out very quickly.

We also tested the procedure on the one-dimensional Ising chain with $b = 3$ where, for low temperatures, exact results[7] give

$$1/T_1 - 1/T_2 = \tfrac{1}{2} \ln b. \tag{5}$$

Our results agree with this equation to within a couple percent. We found matching at $m = 0$, 1, and 2 of an 81-spin chain onto a 27-spin chain. In this calculation and the dynamic calculations described below we used 0.4 million passes for the 81-spin chain and 0.2 million passes for the 27-spin chain.

The Monte Carlo procedure is a kinetic process by its very construction.[8] In the Metropolis sampling procedure the transition probability which determines the dynamics is given by $\min\{\exp(-\delta\mathcal{H}), 1\}$, where $\delta\mathcal{H}$ is the change in the reduced energy induced by flipping the ith spin. We expect this dynamics to be in the same universality class as the Glauber[9] model and our results bear this out. According to the dynamic scaling hypothesis,[10] if the length scales by a fac-

tor of b, then time scales by a factor b^z, where z is the dynamic critical exponent which we wish to compute. The dynamic procedure is similar to that in the static case except that we now compute time-dependent quantities. We chose for reasons of computational simplicity the following:

$$E(N,m,T;t) \equiv (N^{(m)})^{-1}\langle \sum_{\langle ij\rangle} S_i^{(m)}(t)\cdot S_j^{(m)}(0)\rangle_{T,N} \quad (6)$$

and

$$C(N,m,T;t) \equiv (N^{(m)})^{-1}\langle \sum_{i} S_i^{(m)}(t)\cdot S_i^{(m)}(0)\rangle_{T,N}, \quad (7)$$

where the unit of time is one pass through the lattice. The meaning of time in Monte Carlo simulations is reviewed in Ref. 8. From dynamic scaling we expect that after m blockings the time t goes to tb^{mz}. This means that to match time-dependent quantities we must, in addition to finding the temperatures where the static quantities match, find the times such that the time-dependent averages match. In other words we search for the two times t and t' such that

$$E(N,m,T_2,t) = E(Nb^d, m+1, T_1, t'). \quad (8)$$

We can then determine z since $t'/t = b^z$. We carry out a similar procedure for the spin autocorrelation function $C(t)$ defined by Eq. (7).

This method was tested on the 1D Ising chain where exact results[11] give

$$z = -\ln[\tfrac{1}{2}(1-\gamma^2)]/\ln 2, \quad \gamma = \tanh(2/T). \quad (9)$$

We found agreement with this result to within 2% statistical uncertainty for $T_1 = 1.0$ on an 81-spin chain and $T_2 = 0.645$ on a 27-spin chain. Unlike other position-space techniques, the Monte Carlo renormalization-group method treats lattices of all dimensions on the same footing. Since we have obtained excellent agreement in one dimension with the exact value, we expect to obtain reliable results in higher dimensions.

We now discuss our results for the 2D kinetic Ising model. The raw data and the estimates for z based on each quantity are shown in Table I. To

TABLE I. Dynamic Monte Carlo renormalization-group raw data for the two-dimensional kinetic Ising model at temperature $T = T_c$. The quantities E and C are defined in the text. N is number of spins on the lattice, m is the number of blockings, and t is the time. z is the resultant values for the dynamic exponent. z' is the most likely value after subtracting out the slight mismatch for the static quantities $E(N, m, T_c, t = 0)$.

	2^m	N = 256	2^m	N = 64	Z	Z'
E(t=0)						
	1	1.4529±0.0011				
	2	1.4585±0.0037	1	1.49088±0.00058		
	4	1.6059±0.0046	2	1.60393±0.00118		
	8	1.7547±0.0042	4	1.75131±0.00140		
c(t)		t = 40		t = 10		
	1	0.5253±0.0022				
	2	0.6656±0.0027	1	0.62102±0.00062		
	4	0.7678±0.0030	2	0.76257±0.00079	2.24±.16	2.15
	8	0.8474±0.0026	4	0.84120±0.00101	2.27±.14	2.17
E(t)		t = 40		t = 10		
	1	2.100 ± 0.008				
	2	2.659 ± 0.010	1	2.4779 ± 0.0024		
	4	3.060 ± 0.012	2	3.0402 ± 0.0030	2.25±.17	2.23
	8	3.360 ± 0.011	4	3.3457 ± 0.0043	2.18± .16	2.14
c(t)		t = 80		t = 20		
	1	0.5005±0.0030				
	2	0.6389±0.0035	1	0.58838±0.00088		
	4	0.7375±0.0038	2	0.72894±0.00110	2.20±.10	2.15
	8	0.8147±0.0035	4	0.80523±0.00139	2.21±.09	2.13
E(t)		t = 80		t = 20		
	1	2.001 ± 0.012				
	2	2.554 ± 0.014	1	2.3527 ± 0.0035		
	4	2.946 ± 0.016	2	2.9138 ± 0.0045	2.20±.11	2.19
	8	3.251 ± 0.015	4	3.2184 ± 0.0054	2.20±.10	2.18
				average =	2.22±.13	2.17

avoid the necessity of matching static quantities at different temperatures, we used $T_1 = T_2 = T_c$. Because the static quantities match within the statistical error estimates, our procedure gives a T_c in agreement with exact results. For the time-dependent quantities we used times which differ by a factor of 4. If there were perfect matching of the time-dependent quantities then $z = 2$. There is not perfect matching. Using the 64-spin lattice quantities at $t = 10$ and $t = 20$ we can determine how C and E change with time. From this data we can determine for what value of times we would achieve perfect matching. This leads to the first column of z values, which have an average value of $z = 2.22$ with an average 1-standard-deviation uncertainty of 0.13.

We can make a somewhat more informed estimate of z by noting that, if one average in a Monte Carlo simulation fluctuates in one direction, so do all the others. Thus, since our static quantities do not match by some fraction of a standard deviation, the dynamic quantities will also be off by that amount. We can subtract away this part of the error by estimating how much we must change $E(N, m, T_c, t = 0)$, the static quantities, to achieve perfect matching and then make the same percentage change in the time-dependent quantities. This procedure leads to the second column of z estimates in Table I, whose average is $z = 2.17$.

The fact that we have reached the scaling region, i.e., the irrelevant parameters have died out, is confirmed by three facts about the data in Table I, namely that the same values of z within statistical errors are found for (1) two different time-dependent quantities, C and E; (2) two different length scales; and (3) two different time scales. The method can be systematically improved with use of more Monte Carlo passes and/or larger lattices so that more iterations can be performed before matching. It is encouraging, however, that good results are obtained on relatively small lattices.

Results for the dynamic exponent z from other methods vary from $z = 1.4$ to 2.7.[1,12] In these methods the error bars are frequently unknown and systematic improvement is difficult. Our results are closest to those of Achiam, who obtained $z = 2.16$ with use of a real-space renormalization-group method to second order in a cumulant expansion, on a triangular lattice. It is also comparable with the estimate $z = 2.13$ by Racz and Collins based on the high-temperature series expansion of Yahata and Suzuki.[12]

In conclusion, we have developed a novel dynamic Monte Carlo renormalization-group method and applied it successfully to the one- and two-dimensional kinetic Ising model. Our method can be easily extended to any other statistical-mechanical model and offers one of the most reliable means for obtaining information about the dynamic scaling properties of these models. The only limitations are those of access to sufficient computer time. Our procedure can also be used in molecular-dynamics simulations.

We thank G. V. Chester for providing computer time on the Array Processor at Cornell University. This research was in part supported by the National Science Foundation under Grant No. DMR-79-21360 and by the U. S. Air Force Office of Scientific Research under Grant No. 78-3522.

[1]S.-k. Ma, Phys. Rev. Lett. 37, 461 (1976).

[2]R. H. Swendsen, Phys. Rev. Lett. 42, 859 (1979); R. H. Swendsen and S. Krinsky, Phys. Rev. Lett. 43, 177 (1979); H. W. J. Blöte and R. H. Swendsen, Phys. Rev. Lett. 43, 799 (1979).

[3]K. G. Wilson, to be published.

[4]S. Shenker and J. Tobochnik, Phys. Rev. B 22, 4462 (1980).

[5]N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. 21, 1087 (1953).

[6]Th. Niemeijer and J. M. J. van Leeuwen, Physica (Utrecht) 71, 17 (1974).

[7]D. R. Nelson and M. E. Fisher, Ann. Phys. (NY) 91, 226 (1975).

[8]K. Binder and M. H. Kalos, in *Monte Carlo Methods in Statistical Physics*, edited by K. Binder (Springer-Verlag, Berlin, 1979), Chaps. 1 and 6.

[9]R. J. Glauber, J. Math. Phys. 4, 294 (1963).

[10]R. A. Ferrell, N. Monyhard, H. Schmidt, F. Schwabl, and P. Szepfalusy, Ann. Phys. (NY) 47, 565 (1968); B. I. Halperin and P. C. Hohenberg, Phys. Rev. 177, 952 (1969).

[11]Y. Achiam, J. Phys. A 11, 975 (1978).

[12]H. Yahata and M. Suzuki, J. Phys. Soc. Jpn. 27, 1421 (1969); E. Stoll, K. Binder, and T. Schneider, Phys. Rev. B 8, 3266 (1973); H. C. Bolton and C. H. J. Johnson, Phys. Rev. B 13, 3025 (1976); Y. Achiam and J. M. Kosterlitz, Phys. Rev. Lett. 41, 128 (1978); Y. Achiam, J. Phys. A 11, L127 (1978); H. Z. Racz and M. F. Collins, Phys. Rev. B 13, 3074 (1973); M. P. Nightingale and H. W. T. Blöte, Physica (Utrecht) 104A, 352 (1980); G. F. Mazenko, M. J. Nolan, and O. T. Valls, Phys. Rev. B 22, 1275 (1980).