Critical behavior of the two-dimensional random-bond Ising model: A dynamic 1/T expansion

J. D. Reger and A. Zippelius

Institut für Festkörperforschung der Kernforschungsanlage Jülich GmbH, Postfach 1913, D-5170 Jülich, West Germany

(Received 10 December 1984)

We have developed a technique to derive a systematic high-temperature series expansion for dynamic correlations of a random-bond Ising model. Results are presented for the $\pm J$ model in two dimensions. In particular the relaxation rate $\tau_{\rm EA}$ is found to obey an Arrhenius law $\tau_{\rm EA} \sim \exp(\Delta E/T)$ with a finite energy barrier ΔE as $T \rightarrow 0$.

I. INTRODUCTION

The two-dimensional (2D) random-bond Ising model has been the subject of intensive research in recent years. With the help of transfer matrix calculations, Morgenstern and Binder¹ showed that no phase transition occurs at finite temperature. Furthermore, they gave convincing evidence for long-range correlations at T=0. These results were confirmed by extensive Monte Carlo simulations,² which moreover revealed³ a power-law divergence of the correlation length $\xi \sim T^{-\nu}$ and of the spin-glass susceptibility (of Edwards and Anderson) $\chi_{\rm EA} \sim T^{-\gamma}$. Based on these findings, Kinzel and Binder⁴ proposed a simple cluster model to explain their Monte Carlo data and in particular the observed anomalous critical slowing down: The relaxation to equilibrium requires the reorientation of clusters of correlated spins, which have the size of the correlation length ξ . The free-energy barrier ΔE for this process is predicted to diverge as $\Delta E \sim \xi^{(d-1)/2}$ as $T \rightarrow 0$. The relaxation time τ —corresponding to thermal activation—should diverge as $\ln \tau \sim \Delta E/T \sim T^{-\nu z}$ with vz = v(d-1)/2 + 1.

This phenomenological scaling theory was subsequently applied to Monte Carlo data of the $\pm J$ model.^{5,6} A best fit⁶ was obtained with $\gamma = 4.1$, $\nu = 2.75$, and $\nu z = 2$, implying $\Delta E \sim 1/T$. However, the data were found to be consistent also with a finite, but large energy barrier $\Delta E/J \sim 18$. This was first suggested by Morgenstern,⁷ who estimated $\Delta E/J \sim 13$. Using a phenomenlogical renormalization-group approach, McMillan⁸ also predicted finite-energy barriers in agreement with his own Monte

Carlo calculations,⁹ yielding $\Delta E / J \sim 14$. Quite recently McMillan¹⁰ and Bray and Moore¹¹ studied the Ising model with Gaussian bonds at zero temperature. They calculate the energy of defect lines as a function of system size. In d=2 these energies vanish in the thermodynamic limit, $\Delta E_{def} \sim L^{-1/\nu}$ with $\nu=3.56$ and v=3.4, respectively. The nature of these domain walls in a system with frustration and a macroscopic degeneracy of the ground state is not well understood.

To summarize the state of affairs: All studies agree on the absence of a phase transition at finite temperature and, furthermore, that d = 2 is less than the lower critical dimensionality for the random-bond Ising model. However considerable controversy remains as to the critical

behavior at T=0. In particular, the equilibration problems in Monte Carlo calculations are so severe, that the critical behavior must be extrapolated from a temperature range $T/J \sim 1$.

In this paper we present results of a high-temperature series expansion for static and dynamic quantities. For random systems, such studies have previously been restricted to static quantities.^{12,13} The results for d > 4 are considered reliable, whereas the series in dimensions d < 4were found difficult to analyze. As we will show below, the series expansion for dynamic quantities are well behaved and easily analyzed. This allows us to confirm the above scaling ideas in terms of a zero temperature transition. For the dynamic exponent we obtain vz = 1and conclude that the energy barriers are finite as $T \rightarrow 0$.

II. MODEL

We consider an Edwards-Anderson model,¹⁴

$$H_{\rm EA} = -J \sum_{\langle i,j \rangle} \epsilon_{ij} S_i S_j , \qquad (1)$$

for Ising spins of unit length, $S_i^2 = 1$. The exchange energy is a quenched random variable, that fluctuates in sign according to the probability

$$P(\epsilon_{ii}) = p\delta(\epsilon_{ii}-1) + (1-p)\delta(\epsilon_{ii}+1) .$$
⁽²⁾

The model is symmetric around $p = \frac{1}{2}$, so that it is sufficient to consider $\frac{1}{2} \le p \le 1$.

To introduce dynamics, we assume that the system is in contact with a large heat bath giving rise to spontaneous flips of spins.¹⁵ The probability to find the spins in con-figuration $\{S_i\}$ at time t evolves in time according to a Master equation,

$$\partial_t P(S_1, \dots, S_N; t)$$

$$= -\sum_j W_j(S_j) P(S_1, \dots, S_j, \dots, S_N; t)$$

$$+ \sum_i W_j(-S_j) P(S_1, \dots, -S_j, \dots, S_N; t) , \qquad (3)$$

where the probability $W_i(S_i)$ to flip S_i is chosen as

$$W_j(S_j) = \frac{\alpha}{2} \left[1 - S_j \tanh(\beta E_j) \right], \qquad (4)$$

31

5900

$$\beta E_j = K \sum_i \epsilon_{ji} S_i, \quad K = \frac{J}{T} .$$
(5)

In the following we shall set α —the microscopic relaxation rate—equal to 1.

The physical quantities of interest are time-delayed, nonlocal spin correlations,

$$C_{ii}(t) = \langle S_i(0)S_i(t) \rangle .$$
(6)

With help of the Liouville operator,

$$L = \sum_{k} W_{k}(S_{k})(1 - P_{k}) , \qquad (7)$$

these can be represented as

$$C_{ij}(t) = \left\langle S_i(0)e^{-Lt}S_j(0) \right\rangle . \tag{8}$$

The operator P_k flips S_k , according to

$$P_k f(S_1, \ldots, S_k, \ldots, S_N) = f(S_1, \ldots, -S_k, \ldots, S_N) .$$
(9)

The linear-response functions are related to $C_{ij}(t)$ via the fluctuation-dissipation theorem:

$$\chi_{ij}(t) = -\frac{d}{dt} C_{ij}(t), \quad t > 0 .$$
 (10)

Of particular interest are the averaged local susceptibility,

$$\chi(\omega) = \frac{1}{N} \sum_{i} [\chi_{ii}(\omega)]_{av} , \qquad (11)$$

and the Edwards-Anderson susceptibility

$$\chi_{\rm EA}(\omega) = \frac{1}{N} \sum_{i,j,k} [\chi_{ij}(\omega)\chi_{ik}(\omega)]_{\rm av} .$$
⁽¹²⁾

The configurational average with the probability distribution of Eq. (2) has been denoted by $[]_{av}$. In the paramagnetic phase we expect exponential decay for long times. It is then meaningful to define relaxation times as

$$\tau_{q} \equiv -i \frac{\partial \chi^{-1}}{\partial \omega} \bigg|_{\omega=0} = \frac{1}{N} \sum_{i} [\langle S_{i}L^{-1}S_{i} \rangle]_{av}, \qquad (13)$$

$$\tilde{\tau}_{EA} \equiv -i \chi_{EA}(0) \frac{\partial \chi_{EA}^{-1}}{\partial \omega} \bigg|_{\omega=0}$$

$$= 2 \chi_{EA}^{-1}(0) \frac{1}{N} \sum_{i,j,k} [\langle S_{i}L^{-1}S_{j} \rangle \langle S_{i}S_{k} \rangle]_{av} = 2 \frac{\tau_{EA}}{\chi_{EA}}. \qquad (14)$$

These quantities, as well as the static spin-glass susceptibility, have been calculated in a high-temperature series expansion.

III. TECHNIQUE OF THE DYNAMIC 1/T EXPANSION

To set up a dynamic 1/T expansion, we expand the flip rates $W_j(S_j)$ in the number of nearest neighbors, as first suggested by Yahata and Suzuki^{16,17} for a uniform ferromagnet. For the square lattice, this expansion terminates after the second term, yielding the following decomposition of the Liouville operator,

$$L = L_0 - L_1 - L_3 , (15)$$

with

$$L_0 = \frac{1}{2} \sum_k (1 - P_k) , \qquad (16a)$$

$$L_1 = \frac{c_1}{2} \sum_{\langle k,l \rangle} \epsilon_{kl} S_k S_l (1 - P_k) , \qquad (16b)$$

and

$$L_{3} = \frac{c_{3}}{2} \sum_{\langle k, l_{1}, l_{2}, l_{3} \rangle} \epsilon_{k l_{1}} \epsilon_{k l_{2}} \epsilon_{k l_{3}} S_{k} S_{l_{1}} S_{l_{2}} S_{l_{3}} (1 - P_{k}) .$$
(16c)

The summation over l_1, l_2, l_3 in L_3 extends over all nearest neighbors of a given spin S_k with all three of them different. For the particular flip rate of Eq. (4) the coefficients are given by

$$c_1 = \frac{1}{8} (2 \tanh 2K + \tanh 4K) = 0 \left| \frac{1}{T} \right|,$$
 (17a)

$$c_3 = -\frac{1}{8}(2 \tanh 2K - \tanh 4K) = 0 \left[\frac{1}{T^3}\right].$$
 (17b)

To obtain a systematic 1/T expansion we therefore expand the inverse of L in powers of L_1 and L_3 up to the desired order N(M=N/3)

$$L^{-1} = \sum_{n=0}^{M} \left[(L_0 - L_1)^{-1} L_3 \right]^n (L_0 - L_1)^{-1}$$
$$= \sum_{n=0}^{M} \left[L_0^{-1} \sum_{m=0}^{N} (L_1 L_0^{-1})^m L_3 \right]^n$$
$$\times L_3^n L_0^{-1} \sum_{l=0}^{N} (L_1 L_0^{-1})^l .$$
(18)

In the calculation of the relaxation rates [Eqs. (13) and (14)] these operators are applied to a single spin variable S_i , whereby static multispin correlations are generated. These can be calculated in a 1/T expansion by standard methods. Note, however, that we have to keep track of the bond variables, since we are dealing with an inhomogeneous system and the configurational average is the last step in our calculational procedure. A further complication arises, because successive applications of L_3 lead to rather high order static cumulants. For these reasons we have found it more convenient to employ the algorithm of Yahata¹⁷ for the calculation of static cumulants. This algorithm can be implemented on a computer, so that the enumeration of graphs and symmetry factors by hand becomes unnecessary. In that way we were able to obtain ten nontrivial terms for the asymmetric distribution of bonds $(p \neq \frac{1}{2})$ and seven terms for the symmetric distribution. These are listed in Tables I and II.

IV. SERIES ANALYSIS

High-temperature series of the ferromagnetic susceptibility and relaxation rate show,¹⁸ that the ferromagnetic

<u>31</u>

L = 7

L = 8L = 9

L = 10

-

 $3017098 + \frac{2}{3}$

 $3518446 + \frac{14}{27}$

	TABLE 1. Matrix of coefficients a_{lk} for $\tau_{EA} = \sum_{l,k=0} a_{lk} (2p-1) b$ with $b = \tanh(p/1)$.									
	K = 1	K = 2	K = 3	K = 4	K = 5	K = 6	K = 7	K = 8	K = 9	K = 10
L = 0		16		124		$709 + \frac{1}{3}$		$3383 + \frac{5}{9}$		$13331 + \frac{77}{81}$
L = 1	12		148		988		5316		23 020	
L = 2		72		792		4904		24 872		$101417 + \frac{157}{243}$
L=3			360		3780		21 900		$106211 + \frac{19}{27}$	
L = 4				1604		16272		$91735 + \frac{11}{27}$		$436736 + \frac{80}{243}$
L = 5					6492		65 068		$357944 + \frac{4}{9}$	
L = 6						24 704		243 176		1 306 824

89424

TABLE I. Matrix of coefficients a_{lk} for $\tau_{\text{FA}} = \sum_{l,k=0}^{10} a_{lk} (2p-1)^l v^k$ with $v = \tanh J/T$

transition temperature $T_c(p)$ decreases as a function of increasing concentration 1-p of antiferromagnetic bonds. Beyond a critical concentration $p_c \sim 0.85$, no ferromagnetic transition is observed. For higher concentration $\frac{1}{2} \le p \le p_c$, we expect the 2*d* system to undergo a zero temperature transition to a spin-glass phase. In this paper we concentrate on the spin-glass transition and postpone a discussion of the ferromagnetic transition for $p \ge p_c$ to a future publication.¹⁸

The natural expansion variable of the kinetic Ising model is $v(T) = \tanh(J/T)$. If there is a transition at finite temperature the transformation v(T) is analytic and an algebraic singularity in $T - T_c$ is transformed into an algebraic singularity in $|v - v_c|$. However at T = 0 the transformation v(T) is singular and an algebraic singularity in v corresponds to an essential singularity in T. It is therefore very important to choose the correct expansion variable for a zero-temperature transition. For $p \neq \frac{1}{2}$ we have employed the following transformations:

$$v_M(T) = \tanh\left[\sum_{m=1}^M K^m\right] \rightarrow 1 - 2e^{-2K^M} \text{ as } K \rightarrow \infty , \quad (19)$$

$$x(T) = \frac{1}{1 + T/J} \to 1 - T/J \text{ as } T \to 0$$
. (20)

In order to convert the series, for example

TABLE II. Coefficients b_n and c_n for $\tau_q = \sum_{n=0}^7 b_n v^{2n}$ and $\tau_{\text{EA}} = \sum_{n=0}^7 c_n v^{2n}$ for $p = \frac{1}{2}$ and $v = \tanh J/T$.

n	$ au_q(v^{2n})$	$\tau_{\rm EA}(v^{2n})$
1	8	16
2	32	124
3	$\frac{376}{3}$	<u>2128</u> <u>3</u>
4	<u>3392</u> 9	<u>30452</u> 9
5	<u>91976</u> 81	<u>1079888</u> 81
6	<u>3 595 936</u> 1215	<u>59 777 356</u> 1215
7	<u>131 126 104</u> 19 683	73 606 232 656 492 075

 $\tau_{\text{EA}}(v) \rightarrow \tau_{\text{EA}}(x)$, it is a necessary condition that the transformations [(19) and (20)] can be expanded in a power series around 1/T=0.

 $872330 + \frac{2}{9}$

1061068

For $\tau_{\rm EA}$ we assume an essential singularity

312 908

$$\tau_{\rm EA} = \tau_0 e^{\Delta E/T} \tag{21}$$

and allow for a diverging energy barrier $\Delta E/T \sim T^{-vz}$. If the barriers are *finite* as predicted by McMillan, this corresponds to an algebraic singularity in $v = v_1$,

$$\tau_{\rm EA} = \tilde{\tau}_0 |v_1 - 1|^{-\Delta E/2} .$$
(22)

If the energy barriers diverge as $\Delta E \sim b/T$, then Eq. (21) implies an algebraic singularity in $v_{M=2}$,

$$\tau_{\rm EA} = \tau_0' | v_2 - 1 |^{-b/2} . \tag{23}$$

We have analyzed our data with the help of ratio methods as well as Padé approximants. A ratio plot for $\tau_{\rm EA}(v_1) = \sum_{n=0}^{10} a_n v_1^n$ is shown in Fig. 1 for p=0.65. For p close to, but strictly larger than 0.5, the coefficients oscillate, so that it is advantageous to consider the ratios,



FIG. 1. Ratio of coefficients $\mu_{n+1} \equiv (a_{n+1}/a_{n-1})^{1/2} = \mu^* [1 + \Delta E/2n + O(1/n^2)]$ for $\tau_{\text{EA}}(v, p = 0.65) = \sum_{n=0}^{10} a_n v^n$ plotted versus 1/n. The full line shows our estimate of the asymptotic behavior.

$$\mu_{n+1} = \left[\frac{a_{n+1}}{a_{n-1}}\right]^{1/2} \simeq v_1^* \left[1 + \frac{\Delta E}{2n} + O\left[\frac{1}{n^2}\right]\right]. \quad (24)$$

Plotted versus 1/n, these should extrapolate for large n to $v_1^* = 1$ with slope $\Delta E/2$. As can be seen from Fig. 1, the variation of μ_n with 1/n is quite regular for $n \ge 4$. All other expansion variables $v_M(T)$ yield highly erratic series. We interpret this result in the following way: The ratio method fails for v_M ($M \ne 1$), because the assumed form of the singularity of τ_{EA} is incorrect. We find in particular for M=2, that our data are not consistent with $\Delta E \sim 1/T$. So the ratio plots definitely discriminate between various types of singularities for τ_{EA} . However, ten terms are not sufficient to determine the numerical value of ΔE accurately. We estimate $\Delta E \sim 20J$, but note that we are not yet in the asymptotic regime, as can be seen from the curvature of the plot in Fig. 1.

We therefore employ Padé approximants to analyze our data further. As a first step we check our conclusion, that the energy barriers remain finite as $T \rightarrow 0$. This can be done with a Padé analysis for

$$\frac{d\ln[\ln\tau_{\rm EA}(x)]}{dx} = \frac{P_L(x)}{Q_M(x)} \to \frac{-\nu z}{x^* - x} \text{ as } x \to x^*.$$

At the critical point $x^* = 1$ ($T_c = 0$), this function should have a simple pole with residue -vz. The results of an unbiased Padé approximant are listed in Table III for p=0.55. The upper number gives the critical temperature [(we have performed an Euler transformation $x \Longrightarrow x/(1+9x)$, so that the critical point is shifted from $x^*=1 \rightarrow x^*=0.1$)] and the lower number the exponent.

In the Padé analysis we can impose the exact value of $T_c = 0$. The results of such a biased Padé analysis for the exponent vz are shown in Table IV. The upper number refers to an approximant in which the transformation $v \rightarrow x(v)$ was performed before the logarithm of τ_{EA} was taken, and the lower number to the reversed order of transformations. The deviations give an estimate of the error bars involved.

Both types of analysis clearly support the conclusion that ΔE remains finite as $T \rightarrow 0$. Given these results we

TABLE III. Padé table for $d \ln[\ln\tau_{\rm EA}(x)]/dx = P_L(x)/Q_M(x)$ with $x = (1+T/J)^{-1}$; A dash denotes a Padé approximant, which locates another pole on the real axis, close to the physical one; asterisks denote a Padé approximant with a spurious pole. The upper number gives the critical temperature (exact value $x^*=0.1$) and the lower number the exponent vz. The concentration p was chosen as p=0.55.

M	2	3	4	5
2	0.105	0.105	0.098*	0.097
2	1.05	1.05	0.96*	0.95
2	0.105	0.105*	0.097	
3	1.03	1.06*	0.95	
	0.104	0.106*	0.095	
4	0.97	1.10*	0.92	
-		0.109*		
2		1.17*		

TABLE IV. Same as Table III, but with the exact critical temperature imposed. In each entry both numbers refer to the exponent; the upper one to a Padé approximant, in which the transformation $v \rightarrow x(v)$ was performed before the logarithm was taken, and the lower one to the reversed order of transformations.

	2	3	4	5
		0.95	0.96	0.98
2	1.15	1.13	1.15	1.15
2		0.96	0.92*	
3	1.15	1.15		
		0.98		
4	1.14	1.15		
5	0.79	1.01		
5	1.15	1.16		

can determine ΔE from a Padé analysis for $\ln \tau_{EA}(x)$, which should have a simple pole at x^* ,

$$\ln \tau_{\rm EA} \sim \frac{\Delta E}{\mid x^* - x \mid}$$

with residue ΔE . The results of an unbiased Padé approximant are given in Table V. The upper number refers to the critical temperature and the lower number to the energy barrier. The entries in Tables III to V refer to p=0.55, but should be considered typical for $0.5 . We did not observe any significant variation of <math>\Delta E$ with p for $0.55 \le p \le 0.75$.

For $p = \frac{1}{2}$ we have analyzed the data for τ_q and τ_{EA} by ratio methods as well as Padé approximants. The conclusions are qualitatively the same as for $p \neq \frac{1}{2}$, although the limited number of terms does not allow for precise estimates. Nevertheless one feature seems to emerge unambigously: From the data of τ_q and τ_{EA} , we deduce different numerical values for the energy barriers. We are not aware of any argument, that relates the critical singularities of these two dynamic quantities beyond mean-field theory.¹⁹

The dynamic 1/T expansion also provides us with static quantities. Of particular interest is the Edwards-

TABLE V. Padé table for $\ln \tau_{EA}(x)$; the upper number refers to the critical temperature (exact value $x^*=0.1$) and the lower number to the energy barrier $\Delta E / J$.

SM .	2	2	1	5	6
	2	3	4	5	0
2		0.105 18.8	0.104 18.0	0.104 17.9	0.105* 18.1
3	0.105 18.8	0.100 15.5	0.100 15.5	0.099 15.4	0.099 15.2
4	0.104 17.9	0.100 15.5		-	1
5	0.104 17.8	0.099 15.4	-		
6	0.104* 18.1	0.099 15.2			

	K = 1	K = 2	K = 3	K = 4	K = 5	K = 6	K = 7	K = 8	K = 9	K = 10
L = 0		4		12		36		52		116
L = 1	8		24		72		152		264	
L = 2		36		96		248		448		592
L = 3			144		344		808		1000	
L = 4				524		1184		2552		1648
L = 5					1800		3880		7048	
L = 6						5916		11888		18 560
L = 7							18 848		36 072	÷
L=8			-					58 812		104 608
L = 9									179 784	
L = 10										542 452

TABLE VI. Matrix of coefficients b_{lk} for $\chi_{EA} = \sum_{l,k=0}^{10} b_{lk} (2p-1)^l v^k$, with $v = \tanh J/T$.

Anderson susceptibility $\chi_{\rm EA} = \chi_{\rm EA}(\omega = 0)$. The coefficients of the series expansion $\chi_{\rm EA} = \sum_{l,k=0}^{10} b_{lk}(2p-1)^l v^k$ are listed in Table VI. These have been previously calculated by Rajan and Riseborough¹³ up to $l,k \leq 6$. Our results agree, except for the entry b_{55} .

A ratio plot of $\chi_{EA}(v)$ is well behaved and extrapolates to a finite limit as $v \rightarrow 1$. This result confirms the finding of various other authors,¹⁻¹¹ that there is no phase transition at finite temperature. We furthermore conclude, that $\chi_{EA}(T)$ does not have an essential singularity as $T \rightarrow 0$. Our data are consistent with an algebraic singularity $\chi_{EA}(T) \sim T^{-\gamma}$, but not sufficient to provide a reliable estimate of the exponent γ .

ACKNOWLEDGMENT

It is a pleasure to thank K. Binder for many helpful discussions and suggestions and R. G. Palmer for help in the Padé analysis.

- ¹I. Morgenstern and K. Binder, Phys. Rev. Lett. **43**, 1615 (1979); Phys. Rev. B **22**, 288 (1980).
- ²A. P. Young, Phys. Rev. Lett. 50, 917 (1983).
- ³K. Binder, Z. Phys. B 48, 319 (1982).
- ⁴W. Kinzel and K. Binder, Phys. Rev. B 29, 1300 (1984).
- ⁵K. Binder and A. P. Young, Phys. Rev. B 29, 2864 (1984).
- ⁶A. P. Young, J. Phys. C 18, L517 (1984).
- ⁷I. Morgenstern, Phys. Rev. B 27, 4522 (1983).
- ⁸W. L. McMillan, J. Phys. C 17, 3179 (1984).
- ⁹W. L. McMillan, Phys. Rev. B 28, 5216 (1983).
- ¹⁰W. L. McMillan, Phys. Rev. B 29, 4026 (1984).
- ¹¹A. J. Bray and M. A. Moore, J. Phys. C 17, L463 (1984).
- ¹²R. Fisch and A. B. Harris, Phys. Rev. Lett. 38, 785 (1977); D.

- C. Rapaport, J. Phys. C 10, L543 (1977); J. R. Cherry and C. Domb, J. Phys. A 11, L5 (1978); R. V. Ditzian and L. P. Kadanoff, Phys. Rev. B 19, 4631 (1979); R. G. Palmer and F. T. Bantilan (unpublished).
- ¹³V. T. Rajan and P. S. Riseborough, Phys. Rev. B 27, 532 (1983).
- ¹⁴S. F. Edwards and P. W. Anderson, J. Phys. F 5, 965 (1975).
- ¹⁵R. J. Glauber, J. Math. Phys. 4, 294 (1963).
- ¹⁶H. Yahata and M. Suzuki, J. Phys. Soc. Jpn. 27, 1421 (1969).
- ¹⁷H. Yahata, J. Phys. Soc. Jpn. 30, 657 (1971).
- ¹⁸J. D. Reger and A. Zippelius (unpublished).
- ¹⁹H. Sompolinsky and A. Zippelius, Phys. Rev. Lett. **50**, 1297 (1983); A. Zippelius, Phys. Rev. B **29**, 2717 (1984).