Relaxation Times in a Finite Ising System with Random Impurities

K. Oerding¹

Received March 16, 1994; Final July 20, 1994

Finite-size scaling effects of the Ising model with quenched random impurities are studied, focusing on critical dynamics. In contrast to the pure Ising model, disordered systems are characterized by continuous relaxation time spectra. Dynamic field theory is applied to compute the spectral densities of the magnetization M(t) and of $M^2(t)$. In addition, universal cumulant ratios are calculated to second order in $\varepsilon^{1/4}$, where $\varepsilon = 4 - d$ and d < 4 denotes the spatial dimension.

KEY WORDS: Dynamic critical phenomena; disordered spin systems; Ising model; finite size; scaling.

1. INTRODUCTION

During the last few years the critical behavior of disordered Ising systems has recovered much of its early interest. Critical exponents in three dimensions have been calculated to four-loop order⁽¹⁾ and logarithmic corrections in the upper critical dimension have been studied.⁽²⁾ Extensive computer simulations of the dilute Ising model at various concentrations have shown the importance of crossover effects which give rise to effective (nonasymptotic) critical exponents.⁽³⁻⁵⁾ The calculation of these exponents in a field-theoretic renormalization group appraoch requires the study of the flow of the coupling constants away from the fixed points.⁽⁶⁾

In this work finite-size scaling effects of the Ising model with random impurities are investigated to second order in $\varepsilon^{1/4}$ ($\varepsilon = 4 - d$). Since its introduction by Fisher⁽⁷⁾ the idea of finite-size scaling has provided a systematic extrapolation procedure for data obtained by simulations on small samples. An analytic approach to the calculation of finite-size effects

¹ Institut für Theoretische Physik III, Heinrich-Heine-Universität, 40225 Düsseldorf, Germany.

has been developed by Brézin and Zinn-Justin⁽⁸⁾ and extended to critical dynamics by several authors.⁽⁹⁻¹³⁾ The central idea developed in these papers is the derivation of an effective Hamiltonian (or an effective Fokker–Planck equation in the dynamic case) for the homogeneous mode of the order parameter field. This effective Hamiltonian allows the application of nonperturbative methods to obtain correlation functions of the homogeneous mode which cannot be calculated in an expansion around the Gaussian model.

Dynamical properties of a system are determined by relaxation times. Consider, e.g., the normalized correlation function of a quantity \mathscr{A} :

$$\phi_{\mathscr{A}}(t-t') = \frac{\langle \mathscr{A}(t) \mathscr{A}(t') \rangle - \langle \mathscr{A}(t) \rangle \langle \mathscr{A}(t') \rangle}{\langle \mathscr{A}(t)^2 \rangle - \langle \mathscr{A}(t) \rangle^2} \tag{1}$$

For a pure system $\phi_{\mathcal{A}}(t)$ may be written in the form of a series⁽⁹⁾

$$\phi_{\mathcal{A}}(t) = \sum_{n=1}^{\infty} c_{\mathcal{A},n} e^{-|t|/\tau_n}$$
(2)

with a discrete set of relaxation times $\tau_n > 0$. In the limit $t \to \infty$ the correlation function is governed by the contribution with the largest relaxation time and a nonvanishing coefficient $c_{sd,n}$.

In order to compute the relaxation time spectrum of a disordered system one has to perform configurational averages of correlation functions. For an analytical approach it is convenient to average numerator and denominator of ϕ_{ss} separately with respect to disorder instead of averaging the quotient:

$$\phi_{\mathscr{A}}(t-t') = \frac{\overline{\langle \mathscr{A}(t) \mathscr{A}(t') \rangle} - \overline{\langle \mathscr{A}(t) \rangle \langle \mathscr{A}(t') \rangle}}{\overline{\langle \mathscr{A}(t)^2 \rangle} - \overline{\langle \mathscr{A}(t) \rangle^2}}$$
(3)

(Throughout the text, the bar denotes the average over disorder.) This definition differs from the one used in ref. 5. Disorder generates a continuous spectrum of relaxation times which may be described by a density $\rho_{\mathscr{A}}$:

$$\Phi_{\mathcal{A}}(t) = \int_0^\infty d\tau \,\rho_{\mathcal{A}}(\tau) \,e^{-|t|/\tau} \tag{4}$$

The aim of this article is the calculation of $\rho_{sf}(\tau)$ by means of dynamic field theory.⁽¹⁴⁻¹⁶⁾ Section 2 presents the field-theoretic model for an Ising system with random impurities and reviews its renormalization. In Section 3 an effective dynamic functional for the homogeneous mode is derived and an

equivalent formulation of the dynamics by a Fokker-Planck equation is discussed. As a first application of the formalism universal cumulant ratios which may be compared with results obtained by simulations are calculated in Section 4. In Section 5 the spectral densities $\rho_{\mathscr{A}}(\tau)$ for $\mathscr{A} = M$ (magnetization) and $\mathscr{A} = M^2$ are computed. The results are discussed in Section 6.

2. THE MODEL

A field-theoretic model for a system with quenched random impurities is given by the Landau–Ginzburg Hamiltonian

$$\mathscr{H}_{\psi}[s] = \int d^{d}r \left[\frac{\tau}{2} s^{2} + \frac{1}{2} (\nabla s)^{2} + \frac{g}{4!} s^{4} + \frac{1}{2} \psi s^{2} \right]$$
(5)

where s is an order parameter field and ψ models the impurities which shift the temperature locally. In this paper we consider an (n=1)-component order parameter (Ising model), since for $n \ge 2$ the specific heat exponent is negative (for d=3) and the impurities are irrelevant for the asymptotic critical behavior.⁽¹⁷⁾ The distribution of the random field ψ is Gaussian with zero mean and the correlations

$$\overline{\psi(\mathbf{r})}\,\overline{\psi(\mathbf{r}')} = f\delta(\mathbf{r} - \mathbf{r}') \tag{6}$$

The dynamics of a nonconserved order parameter can be expressed in the form of the Langevin equation

$$\partial_{t}s = -\lambda \frac{\partial \mathscr{H}_{\psi}[s]}{\delta s(\mathbf{r}, t)} + \zeta(\mathbf{r}, t)$$
(7)

where ζ is a Gaussian random force which models the microscopic degrees of freedom:

$$\langle \zeta(\mathbf{r}, t) \zeta(\mathbf{r}', t') \rangle = 2\lambda \delta(\mathbf{r} - \mathbf{r}') \delta(t - t')$$
 (8)

(The brackets $\langle \cdots \rangle$ denote an average over thermal noise.) In the sequel a path integral formalism is employed which is equivalent to the Langevin equation (7) but better suited for the application of field-theoretic renormalization-group methods. Mean values are obtained as functional averages with weight $\exp(-\mathcal{T}_{\psi}[\tilde{s}, s])$, where \mathcal{T}_{ψ} is the dynamic functional⁽¹⁴⁻¹⁶⁾

$$\mathscr{T}_{\psi}[\tilde{s},s] = \int dt \int d^{d}r \left[\tilde{s} \left(\partial_{\tau} s + \lambda(\tau - \Delta)s + \frac{\lambda g}{6} s^{3} + \lambda \psi s \right) - \lambda \tilde{s}^{2} \right]$$
(9)

The response field \tilde{s} has been introduced to average over the thermal noise. Since the weight $\exp(\mathcal{T}_{\psi})$ requires no ψ -dependent normalization constant, one may average over ψ without introducing replicas⁽¹⁸⁾

$$\overline{\exp(-\mathscr{T}_{\psi}[\tilde{s},s])} = \exp(-\mathscr{T}[\tilde{s},s])$$
(10)

where

$$\mathcal{F}[\tilde{s}, s] = \int d^{d}r \left[\int dt \left(\tilde{s} \left(\partial_{\tau} s + \lambda(\tau - \Delta) s + \frac{\lambda g}{6} s^{3} \right) - \lambda \tilde{s}^{2} \right) - \frac{\lambda^{2} f}{2} \left(\int dt \, \tilde{s} s \right)^{2} \right]$$
(11)

A perturbative calculation of correlation and response functions (treating the coupling coefficients f and g as perturbations) leads to integrals which are ultraviolet-divergent at the upper critical dimension $d_c = 4$. To obtain a well-defined renormalized field theory we render these integrals finite by analytic continuation in d (dimensional regularization) and absorb the remaining poles at $\varepsilon = 0$ into renormalizations of coupling constants and fields. The required renormalization constants have been calculated at two-loop order.^(6,19) Here only the one-loop Z-factors are shown, since they are sufficient for our purpose. The renormalizations are

$$\tilde{s} \to \tilde{s}_0 = Z_{\tilde{s}}^{1/2} \tilde{s} \qquad s \to s_0 = Z_{\tilde{s}}^{1/2} s$$

$$\tau \to \tau_0 = (Z_{\tau}/Z_s)\tau \qquad \lambda \to \lambda_0 = (Z_s/Z_{\tilde{s}})^{1/2} \lambda$$

$$g \to g_0 = (Z_u/Z_s^2)g \qquad f \to f_0 = (Z_v/Z_s^2)f$$

$$G_s g = u\mu^s \qquad G_s f = v\mu^s$$
(12)

where the bare quantities are indicated by the index 0, and

$$Z_{\overline{s}} = 1 - (4v)/\varepsilon + \cdots \qquad Z_{s} = 1 + \cdots$$

$$Z_{\tau} = 1 + u/\varepsilon - (2v)/\varepsilon + \cdots \qquad Z_{u} = 1 + (3u)/\varepsilon - (12v)/\varepsilon + \cdots \quad (13)$$

$$Z_{v} = 1 + (2u)/\varepsilon - (8v)/\varepsilon + \cdots$$

In (12), μ is an external momentum scale and the factor $G_{\varepsilon} = \Gamma(1 + \varepsilon/2)/(4\pi)^{d/2}$ has been introduced for convenience.

3. EFFECTIVE FUNCTIONAL FOR THE q = 0 MODE

In this section the model (11) is considered in a finite cubic geometry of linear size L with periodic boundary conditions. The calculation of finite-size effects in this field theory follows the line taken in the analysis of the finite pure system⁽⁹⁻¹¹⁾ and the discussion of nonequilibrium phase transitions in a finite geometry.^(12,13)

We transform the fields \tilde{s}_0 and s_0 to Fourier space by writing

$$\tilde{s}_0(\mathbf{r}, t) = \sum_{\mathbf{q}} \tilde{s}_{0,\mathbf{q}}(t) e^{i\mathbf{q}\mathbf{r}}, \qquad s_0(\mathbf{r}, t) = \sum_{\mathbf{q}} s_{0,\mathbf{q}}(t) e^{i\mathbf{q}\mathbf{r}}$$
(14)

where $q_{\alpha} = (2\pi/L) n_{\alpha}$, $n_{\alpha} = 0, \pm 1, \pm 2, ..., (\alpha = 1, ..., d)$. At the critical point the q = 0 modes may not be treated perturbatively, since the correlator of the field s has an isolated pole at $q^2 = 0$. Additional factors of the form $1/q^2$ are generated through time integrations in Feynman graphs. In order to treat the q = 0 modes separately we decompose the fields \tilde{s}_0 , s_0 into homogeneous modes $\tilde{M}_0(t)$, $M_0(t)$ and their orthogonal complements $\tilde{\phi}_0((\tilde{\phi}_0 \mathbf{r}, t), \phi_0(\mathbf{r}, t))$:

$$\tilde{s}_{0}(\mathbf{r}, t) = \tilde{M}_{0}(t) + \tilde{\phi}_{0}(\mathbf{r}, t) \qquad \tilde{M}_{0}(t) = L^{-d} \int d^{d}r \, \tilde{s}_{0}(\mathbf{r}, t)$$

$$s_{0}(\mathbf{r}, t) = M_{0}(t) + \phi_{0}(\mathbf{r}, t) \qquad M_{0}(t) = L^{-d} \int d^{d}r \, s_{0}(\mathbf{r}, t)$$
(15)

One obtains an effective dynamical action $\mathscr{T}_{hom}[\tilde{M}_0, M_0]$ by integrating out all $q \neq 0$ modes:

$$\exp(-\mathcal{T}_{hom}[\tilde{M}_0, M_0])$$

$$= \int \mathcal{D}[\tilde{\phi}_0, \phi_0] \exp(-\mathcal{T}[\tilde{M}_0 + \tilde{\phi}_0, M_0 + \phi_0])$$

$$= \int \mathcal{D}[\tilde{\phi}_0, \phi_0] \exp(-\mathcal{T}_{hom}^{(0)}[\tilde{M}_0, M_0] - \mathcal{T}_G[\tilde{\phi}_0, \phi_0]$$

$$-\mathcal{T}_{int}[\tilde{M}_0, M_0; \tilde{\phi}_0, \phi_0])$$

where

$$\mathcal{F}_{\text{hom}}^{(0)}[\tilde{M}_0, M_0] = L^d \left[\int dt \left(\tilde{M}_0 \left(\partial_I M_0 + \lambda_0 \tau_0 M_0 + \frac{\lambda_0 g_0}{6} M_0^3 \right) - \lambda_0 \tilde{M}_0^2 \right) - \frac{\lambda_0^2 f_0}{2} \left(\int dt \; \tilde{M}_0 M_0 \right)^2 \right]$$
(16)

$$\mathscr{T}_{G}[\widetilde{\phi}_{0},\phi_{0}] = \int d^{d}r \int dt [\widetilde{\phi}_{0}(\partial_{t}\phi_{0} + \lambda_{0}(\tau_{0} - \Delta)\phi_{0}) - \lambda_{0}\widetilde{\phi}_{0}^{2}]$$
(17)



Fig. 1. One-loop contributions to \mathcal{F}_{hom} [Eq. (24)]. Wiggly lines with or without an arrow represent \tilde{M} or M fields, respectively; broken lines represent correlations of the disorder.

and

$$\mathcal{F}_{int}[\tilde{M}_{0}, M_{0}; \tilde{\phi}_{0}, \phi_{0}]$$

$$= \int d^{d}r \left\{ \int dt \left(\frac{\lambda_{0} g_{0}}{2} M_{0}^{2} \tilde{\phi}_{0} \phi_{0} + \frac{\lambda_{0} g_{0}}{2} \tilde{M}_{0} M_{0} \phi_{0}^{2} \right) \right.$$

$$\left. - \lambda_{0}^{2} f_{0} \left[\left(\int dt \tilde{M}_{0} M_{0} \right) \left(\int dt \tilde{\phi}_{0} \phi_{0} \right) \right.$$

$$\left. + \left(\int dt \tilde{M}_{0} \phi_{0} \right) \left(\int dt \tilde{\phi}_{0} M_{0} \right) \right.$$

$$\left. + \frac{1}{2} \left(\int dt \tilde{M}_{0} \phi_{0} \right)^{2} + \frac{1}{2} \left(\int dt \tilde{\phi}_{0} M_{0} \right)^{2} \right] \right\} + \cdots \qquad (18)$$

In Eq. (18), only those interactions are given which are necessary to calculate the leading contributions to \mathcal{T}_{hom} for small ε (this statement will be explained below). The Feynman graphs which have to be evaluated to obtain the shift of T_c and the renormalization of coupling constants are shown in Fig. 1.

To see what calculation has to be performed to derive the effective functional, let us consider the second graph in the first row of Fig. 1 in more detail. Its contribution to \mathcal{T}_{hom} reads

$$\lambda_{0}^{2} f_{0} \int_{-\infty}^{\infty} dt \int_{-\infty}^{t} dt' \, \tilde{M}_{0}(t) \, M_{0}(t') \, L^{-d} \sum_{\mathbf{q} \neq \mathbf{0}} e^{-\lambda_{0}(\tau_{0} + q^{2})(t - t')}$$
(19)

Using the Taylor series

$$M_0(t') = \sum_{j=0}^{\infty} \frac{1}{j!} M_0^{(j)}(t)(t'-t)^j$$
(20)

one obtains the expansion

$$(19) = \lambda_0 f_0 \int_{-\infty}^{\infty} dt \, \tilde{M}_0(t) \sum_{j=0}^{\infty} \frac{(-\lambda_0)^{-j}}{j!} M_0^{(j)}(t) \, L^{-d} \sum_{q \neq 0} \frac{1}{(\tau_0 + q^2)^{j+1}}$$
$$= \lambda_0 f_0 \int_{-\infty}^{\infty} dt \, \tilde{M}_0(t) \left(\frac{L}{2\pi}\right)^{2-d}$$
$$\times \sum_{j=0}^{\infty} \frac{1}{(j!)^2} \left(\frac{L^2}{4\pi^2 \lambda_0}\right)^j M_0^{(j)}(t) \, I^{(j)} \left(\tau_0 \left(\frac{L}{2\pi}\right)^2\right)$$
(21)

where the function I(x) is defined as a d-dimensional sum over integers

$$I(x) = \frac{1}{(2\pi)^d} \sum_{n \neq 0} \frac{1}{x + n^2}$$
(22)

As mentioned above, the bare parameters and fields have to be expressed by their renormalized counterparts τ , λ , f, g, \tilde{M} , and M to remove ultraviolet divergences from the theory. The divergencies in the expansin (21) come from the functions I(x) and I'(x). We will return to this point later in this section.

The next step is to decide which terms in the expansion have to be kept to obtain physical quantities at second order in $\varepsilon^{1/4}$. For this purpose it is crucial to realize that the interaction $\int dt \tilde{M}M^3$ has to be present already at lowest order in the perturbation series since it is required to stabilize the system at temperatures $T \leq T_c$. (Remember that above four dimensions g_0 is a dangerous irrelevant variable.) On the other hand, the renormalized coupling constant g is at the random fixed point of order $\varepsilon^{1/2}$.⁽¹⁹⁾ In order to see how the expansion in (noninteger) powers of ε is organized we rescale \tilde{M} , M, and t in such a way that the coefficient of $\int dt \tilde{M}M^3$ becomes $O(\varepsilon^0)$ at the fixed point of the renormalized theory while the Gaussian part remains unchanged for $\tau = 0$:

$$\tilde{M} \to \varepsilon^{1/8} \tilde{M}, \qquad M \to \varepsilon^{-1/8} M, \qquad t \to \varepsilon^{-1/4} t$$
 (23)

Inserting these rescalings into the expansion (21) and remembering that $f = O(\varepsilon^{1/2})$ at the fixed point one, finds that the leading term (j=0) is of order $\varepsilon^{1/4}$, while the second term (j=1) is of order $\varepsilon^{1/2}$. All other contributions are at least $O(\varepsilon^{3/4})$.

In the same way one can make sure that all other new interactions (not contained in $\mathscr{T}_{hom}^{(0)}$) can be ignored at order $\varepsilon^{1/2}$. The same is true for contributions from diagrams with more than one loop.

After these considerations the calculation yields the effective functional

$$\mathcal{T}_{\text{hom}}[\tilde{M}_0, M_0] = L^d \left[\int dt \left(\tilde{M}_0 \left(\hat{r}_0 \partial_\tau M_0 + \lambda_0 \hat{\tau}_0 M_0 + \frac{\lambda_0 \hat{g}_0}{6} M_0^3 \right) - \lambda_0 \hat{r}_0 \tilde{M}_0^2 \right) - \frac{1}{2} \lambda_0^2 \hat{f}_0 \left(\int dt \, \tilde{M}_0 M_0 \right)^2 \right]$$
(24)

where

$$\hat{\tau}_{0} = \tau_{0} + \left(\frac{1}{2}g_{0} - f_{0}\right)\left(\frac{L}{2\pi}\right)^{-(d-2)} I\left(\tau_{0}\left(\frac{L}{2\pi}\right)^{2}\right)$$

$$\hat{g}_{0} = g_{0}\left(1 + \frac{3}{2}(g_{0} - 4f_{0})\left(\frac{L}{2\pi}\right)^{4-d} I'\left(\tau_{0}\left(\frac{L}{2\pi}\right)^{2}\right)\right)$$

$$\hat{f}_{0} = f_{0}\left(1 + (g_{0} - 4f_{0})\left(\frac{L}{2\pi}\right)^{4-d} I'\left(\tau_{0}\left(\frac{L}{2\pi}\right)^{2}\right)\right)$$

$$\hat{r}_{0} = 1 - f_{0}\left(\frac{L}{2\pi}\right)^{4-d} I'\left(\tau_{0}\left(\frac{L}{2\pi}\right)^{2}\right), \quad \hat{\lambda}_{0} = \lambda_{0}\hat{r}_{0}$$
(25)

The function I(x) may be written in the form

$$I(x) = \frac{1}{(2\pi)^d} \sum_{\mathbf{n} \neq 0} \frac{1}{x + \mathbf{n}^2} = \frac{1}{(2\pi)^d} \int_0^\infty dt \ e^{-xt} (A(t)^d - 1)$$
(26)

where

$$A(t) = \sum_{n = -\infty}^{\infty} e^{-n^2 t} = \left(\frac{\pi}{t}\right)^{1/2} A\left(\frac{\pi^2}{t}\right)$$
(27)

Equation (27) (which follows from Poisson's formula⁽²⁰⁾) shows that the integral I(x) diverges for $d \ge 2$. Using dimensional regularization, we get⁽¹²⁾

$$I(x) = G_{\varepsilon}\left(a(x) - \frac{2x}{\varepsilon}\right)$$
(28)

where a(x) is finite for $\varepsilon = 0$. For $\varepsilon = 0$ and x large a(x) behaves as

$$a(x) \simeq x(\ln x - 1) + O(x^0)$$
 (29)

while

$$a(0) = \frac{1}{\pi^2} \int_0^\infty dt \left(A(t)^4 - \left(\frac{\pi}{t}\right)^2 - 1 \right) = -\frac{8 \ln 2}{\pi^2}$$
(30)

The coefficients in the Taylor series for a(x) are given in the appendix of ref. 12.

To obtain a renormalized effective action we insert I(x) [Eq. (28)] into Eqs. (25) and (24) and express the bare couplings and fields by their renormalized counterparts. In this way one finds the effective renormalized couplings

$$\hat{\tau} = \tau \left(1 + \left(\frac{u}{2} - v \right) \left(\frac{a(x)}{x} - 2 \ln \frac{\mu L}{2\pi} \right) \right)$$

$$\hat{g} = g \left(1 + \frac{3}{2} \left(u - 4v \right) \left(a'(x) - \ln \frac{\mu L}{2\pi} \right) \right)$$

$$\hat{f} = f \left(1 + \left(u - 4v \right) \left(a'(x) - \ln \frac{\mu L}{2\pi} \right) \right)$$

$$\hat{r} = 1 - v \left(a'(x) - \ln \frac{\mu L}{2\pi} \right)$$
(31)

where $x = \tau (L/(2\pi))^2$. The scaling behavior of the functions $\hat{\tau}(\tau, L)$, $\hat{g}(\tau, L)$, $\hat{f}(\tau, L)$, and $\hat{r}(\tau, L)$ may be derived from renormalization group equations. At the random-fixed point $u_* = 4(3\epsilon/106)^{1/2}$, $v_* = (3\epsilon/106)^{1/2}$ we obtain

$$\hat{\tau} = \tau \left(\frac{\mu L}{2\pi}\right)^{(1/\nu) + \eta - 2} T(y)$$

$$\hat{g} = g_* \left(\frac{\mu L}{2\pi}\right)^{d - 4 + 2\eta} G(y)$$

$$\hat{f} = f_* \left(\frac{\mu L}{2\pi}\right)^{d - 4 + 2\eta} F(y)$$

$$\hat{r} = \left(\frac{\mu L}{2\pi}\right)^{z - 2 + \eta} R(y)$$
(32)

with the scaling variable $y = (\tau/\mu^2)(\mu L/(2\pi))^{1/\nu}$. Since these functions must become independent of L in the bulk limit $L \to \infty$ we expect the asymptotic behavior

$$\begin{array}{ll} T(y) \sim y^{-1+\nu(2-\eta)} & R(y) \sim y^{-\nu(z-2+\eta)} \\ G(y) \sim y^{\nu(4-d-2\eta)} & F(y) \sim y^{\nu(4-d-2\eta)} \end{array} \text{ for } y \to \infty$$
 (33)

Using $-1 + \nu(2 - \eta) = (3\varepsilon/106) + \cdots$, we may write

$$T(y) = 1 + \left(\frac{3\varepsilon}{106}\right)^{1/2} \frac{a(y)}{y} + O(\varepsilon)$$

= $(1+y)^{-1+\nu(2-\eta)} \left\{ 1 + \left(\frac{3\varepsilon}{106}\right)^{1/2} \left[\frac{a(y)}{y} - \ln(1+y)\right] + O(\varepsilon) \right\}$ (34)

Oerding

which explicitly displays the expected behavior for large y. Analogously, one finds

$$R(y) = (1+y)^{-\nu(z-2+\eta)} \left\{ 1 - \left(\frac{3\varepsilon}{106}\right)^{1/2} \left[a'(y) - \ln(1+y)\right] + O(\varepsilon) \right\}$$
(35)

Note that F(y) and G(y) are trivially $F(y) = 1 + O(\varepsilon)$ and $G(y) = 1 + O(\varepsilon)$ to this order. Since $\eta = O(\varepsilon)$, this is consistent with the limiting behavior (33).

In order to calculate correlation functions for the homogeneous mode M in the finite-size scaling limit one has to perform functional averages with the weight $\exp(-\mathcal{T}_{hom})$, where

$$\mathcal{F}_{hom}[\tilde{M}, M] = L^{d} \left[\int dt \left(\tilde{M} \left(\hat{r} \partial_{\tau} M + \lambda \hat{\tau} M + \frac{\lambda \hat{g}}{6} M^{3} \right) - \lambda \hat{r} \tilde{M}^{2} \right) - \frac{1}{2} \lambda^{2} \hat{f} \left(\int dt \ \tilde{M} M \right)^{2} \right]$$
(36)

Since we are especially interested in relaxation times, it is appropriate to describe the dynamics in the form of a Fokker-Planck equation equivalent to the statistical functional (36). Relaxation rates are then obtained as eigenvalues of the Fokker-Planck operator. However, the derivation of a Fokker-Planck equation is complicated by the presence of the noise term proportional to $(\int dt \tilde{M}M)^2$, which reflects the disorder. This term may be formally removed from \mathscr{T}_{hom} by introducing an auxiliary Gaussian random variable X and an X-dependent dynamic functional \mathscr{T}_X :

$$\exp(-\mathscr{T}_{hom}[\tilde{M}, M]) = \int_{-\infty}^{\infty} \frac{dX}{(2\pi)^{1/2}} \exp\left(-\frac{X^2}{2}\right) \\ \times \exp(-\mathscr{T}_X[\tilde{M}, M])$$
(37)

where

$$\mathcal{T}_{X}[\tilde{M}, M] = L^{d} \int dt \, \tilde{M} \left\{ \hat{r}\partial_{\tau}M + \lambda \left[\hat{\tau} + \left(\frac{\hat{f}}{L^{d}}\right)^{1/2} X \right] M + \frac{\lambda \hat{g}}{6} M^{3} - \lambda \hat{r}\tilde{M} \right\}$$
(38)

The Fokker–Planck equation corresponding to \mathcal{T}_{χ} is given by

$$\frac{\partial}{\partial t} P_X(M, t) = \frac{\lambda}{L^d f} \frac{\partial}{\partial M} \left(H'_X(M) + \frac{\partial}{\partial M} \right) P_X(M, t)$$
(39)

where

$$H_X(M) = L^d \left\{ \frac{1}{2} \left[\hat{\tau} + \left(\frac{\hat{f}}{L^d} \right)^{1/2} X \right] M^2 + \frac{\hat{g}}{4!} M^4 \right\}$$
(40)

We now obtain the correlation functions of interest by averaging X-dependent solutions of Eq. (39) with respect to X, e.g.,

$$\overline{\langle \mathscr{A}(M(t)) \mathscr{A}(M(t')) \rangle} = \int_{-\infty}^{\infty} \frac{dX}{(2\pi)^{1/2}} e^{-X^{2}/2} \langle \mathscr{A}(M(t)) \mathscr{A}(M(t')) \rangle_{X}$$
$$= \int_{-\infty}^{\infty} \frac{dX}{(2\pi)^{1/2}} e^{-X^{2}/2} \int_{-\infty}^{\infty} dM \int_{-\infty}^{\infty} dM' \mathscr{A}(M) \mathscr{A}(M')$$
$$\times P_{X}(M' \to M, t-t') P_{X}^{\infty}(M') \quad \text{for } t > t'$$
(41)

where $P_X^{\infty}(M)$ is the equilibrium distribution $N(X) \exp(-H_X(M))$ and $P_X(M' \to M, t-t')$ denotes a transition probability.

4. UNIVERSAL CUMULANT RATIOS

A useful quantity in the study of critical phenomena by Monte Carlo methods is the cumulant ratio introduced by Binder⁽²¹⁾

$$U = 1 - \frac{\langle M^4 \rangle}{3 \langle M^2 \rangle^2} \tag{42}$$

which depends only on the scaling variable $y \propto \tau L^{1/\nu}$. At the critical point U becomes a universal number which has been calculated for the pure Ising model to second order in $\sqrt{\epsilon}$.⁽⁸⁾

Since in the case of disordered spin systems one has to perform configurational averages, there are three different ratios which may be considered:

$$U_1 = 1 - \frac{\overline{\langle M^4 \rangle}}{3 \,\overline{\langle M^2 \rangle^2}}, \quad U_2 = 1 - \frac{\overline{\langle M^4 \rangle}}{3 \,\overline{\langle M^2 \rangle^2}}, \quad U_3 = 1 - \overline{\left(\frac{\langle M^4 \rangle}{3 \,\overline{\langle M^2 \rangle^2}}\right)}$$
(43)

The formalism presented in the previous section permits a straightforward calculation of U_1 . To compute equal-time averages we do not need to know the transition probability in Eq. (41), but only the equilibrium distribution $P_X^{\infty}(M)$:

$$\overline{\langle \mathscr{A}(M(t))\rangle} = \overline{\langle \mathscr{A}(M)\rangle} = \int_{-\infty}^{\infty} \frac{dX}{(2\pi)^{1/2}} e^{-X^2/2} \int_{-\infty}^{\infty} dM \,\mathscr{A}(M) \, P_X^{\infty}(M) \quad (44)$$

Defining the functions

$$\Gamma_k(x) = \int_{-\infty}^{\infty} dq \ q^{2k} \exp\left(-\frac{x}{2}q^2 - \frac{1}{4!}q^4\right) \quad \text{for} \quad k = 0, 1, 2, \dots \quad (45)$$

$$C_k(x) = \frac{\Gamma_k(x)}{\Gamma_0(x)} \tag{46}$$

one obtains

$$\overline{\langle M^{2k} \rangle} = (\hat{g}L^d)^{-k/2} \int_{-\infty}^{\infty} \frac{dX}{(2\pi)^{1/2}} e^{-X^2/2} C_k \left(\left(\frac{L^d}{\hat{g}} \right)^{1/2} \hat{\tau} + \left(\frac{\hat{f}}{\hat{g}} \right)^{1/2} X \right) \quad (47)$$

This yields for $T = T_c$ at the random-fixed point the universal ratio

$$U_1 = 0.216368 + 0.092017\varepsilon^{1/4} + 0.009625\varepsilon^{1/2} + O(\varepsilon^{3/4})$$
(48)

with the three dimensional estimate $U_1(\varepsilon = 1) = 0.3180$.

To obtain the average $\overline{\langle M^2 \rangle^2}$ or more general correlation functions of the form

$$\overline{\langle M(t_1)^{k_1} \rangle \langle M(t_2)^{k_2} \rangle \cdots \langle M(t_n)^{k_n} \rangle} \qquad (n = 1, 2, ...)$$

we introduce *n* replicas before taking the configurational average. The replica method is necessary at this point because $\langle M^2 \rangle^2$ is a product of two thermal averages which has to be averaged with respect to disorder. Since the thermal expectation values have to be calculated for the same impurity configuration, the average over disorder does not factorize. However, one may use the replica trick to rewrite the product of *n* thermal correlation functions in the form of a single correlation function of *n* different fields. The configurational average can then be performed first. This yields the dynamic functional

$$\mathcal{T}_{n}[\tilde{s}, s] = \int d^{d}r \left[\int dt \sum_{\alpha=1}^{n} \tilde{s}_{\alpha} \left(\partial_{\tau} s_{\alpha} + \lambda(\tau - \Delta) s_{\alpha} + \frac{\lambda g}{6} s_{\alpha}^{3} - \lambda \tilde{s}_{\alpha} \right) - \frac{\lambda^{2} f}{2} \left(\int dt \sum_{\alpha=1}^{n} \tilde{s}_{\alpha} s_{\alpha} \right)^{2} \right]$$
(49)

Taking the trace over $q \neq 0$ modes, one obtains an effective functional for the homogeneous modes \tilde{M}_{α} , M_{α} :

$$\mathcal{T}_{n,\text{hom}}[\tilde{M}, M] = L^{d} \left[\int dt \sum_{\alpha=1}^{n} \tilde{M}_{\alpha} \left(\hat{r} \partial_{\tau} M_{\alpha} + \lambda \hat{\tau} M_{\alpha} + \frac{\lambda \hat{g}}{6} M_{\alpha}^{3} - \lambda \hat{r} \tilde{M}_{\alpha} \right) - \frac{1}{2} \lambda^{2} \hat{f} \left(\int dt \sum_{\alpha=1}^{n} \tilde{M}_{\alpha} M_{\alpha} \right)^{2} \right]$$
(50)

904

As a consequence of causality the functions \hat{r} , $\hat{\tau}$, \hat{g} , and \hat{f} are independent of *n* and thus identical with those given in Eqs. (31), (32). Introducing a single Gaussian random variable X as in Eq. (38), it is easy to show that the distribution of each mode M_{α} satisfies the Fokker-Planck equation (39). Thus the stationary distribution factorizes and the average of $\langle M^2 \rangle^2$ with respect to disorder is given by

$$\overline{\langle M^2 \rangle^2} = (\hat{g}L^d)^{-1} \int_{-\infty}^{\infty} \frac{dX}{(2\pi)^{1/2}} e^{-X^2/2} C_1 \left(\left(\frac{L^d}{\hat{g}} \right)^{1/2} \hat{\tau} + \left(\frac{\hat{f}}{\hat{g}} \right)^{1/2} X \right)^2$$
(51)

Expanding the ratio U_2 at the critical point in powers of $\varepsilon^{1/4}$, we obtain

$$U_2 = 0.401918 + 0.084739\varepsilon^{1/4} - 0.005651\varepsilon^{1/2} + O(\varepsilon^{3/4})$$
(52)

and the three-dimensional estimate $U_2(\varepsilon = 1) = 0.4810$.

To compute the third cumulant ratio U_3 by the replica method, one may extend the average

$$\frac{\overline{\langle M^4 \rangle}}{\langle M^2 \rangle^2} \langle M^2 \rangle^n \qquad (n=2, 3, ...)$$

analytically to a convex function of *n* and then perform the limit $n \rightarrow 0$. This procedure is mathematically not rigorous, since the analytic continuation of a function which is known only for a discrete set of points is not unique. However, a particular way of continuation is suggested by the form of the effective functional (38) and the Hamiltonian (40): To calculate correlation functions of the homogeneous mode at second order in $\varepsilon^{1/4}$ one can replace the *d*-dimensional random field $\psi(\mathbf{r})$ by a single random variable X. Adopting this idea for the calculation of $\langle M^4 \rangle / \langle M^2 \rangle^2$, we obtain

$$\overline{\left(\frac{\langle M^4 \rangle}{\langle M^2 \rangle^2}\right)} = \int_{-\infty}^{\infty} \frac{dX}{(2\pi)^{1/2}} e^{-X^2/2} \frac{C_2((L^d/\hat{g})^{1/2} \hat{\tau} + (\hat{f}/\hat{g})^{1/2} X)}{C_1((L^d/\hat{g})^{1/2} \hat{\tau} + (\hat{f}/\hat{g})^{1/2} X)^2}$$
(53)

At the critical point this gives

$$U_3 = 0.283908 + 0.076024\varepsilon^{1/4} + 0.005347\varepsilon^{1/2} + O(\varepsilon^{3/4})$$
(54)

and the estimate $U_3(\varepsilon = 1) = 0.3653$.

The computer simulation⁽⁴⁾ of a site-disordered Ising system with a concentration p = 0.8 yields $U_3 = 0.48$. The disagreement between the one-loop result and the simulation is probably due to the low accuracy of the $\varepsilon^{1/4}$ expansion for $\varepsilon = 1$. On the other hand, one has to check if the simulation has reached the asymptotic scaling region where exponents and

amplitudes calculated at the random fixed point are valid. Deviations from the asymptotic scaling behavior lead to concentration-dependent effective exponents. The effective exponents obtained in ref. 4 for p = 0.8 are quite close to the fixed-point exponents, but the effective U_3 may depend more sensitively on p than the exponents. Therefore simulations at various concentrations could be helpful. Unfortunately, in ref. 4, U_3 is only given for p = 0.8.

More accurate analytic estimates for the cumulant ratios could probably be obtained at one-loop order from an effective functional in three dimensions (i.e., without the $\varepsilon^{1/4}$ expansion). However, beyond the second order in $\varepsilon^{1/4}$ we lose the justification for ignoring interactions which are not already contained in $\mathcal{F}_{hom}^{(0)}$. One has thus to allow for correlated noise and non-Markovian interactions which are generated by tracing out the $q \neq 0$ modes. Even for the pure system there is no work known to the author where the effective functional for d=3 has been studied.

5. RELAXATION TIME DISTRIBUTIONS

Following an idea of Goldschmidt,⁽²²⁾ it is convenient to transform the Fokker-Planck equation (39) to a Schrödinger equation in imaginary time and calculate eigenvalues approximately by means of a variational method. In order to remove the first-order derivative with respect to M in Eq. (39) we express $P_X(M, t)$ by a "wave function" $\bar{\psi}_X(M, t)$,

$$P_{X}(M, t) = \bar{\psi}_{X}(M, t) \exp[-\frac{1}{2}H_{X}(M)]$$
(55)

and obtain

$$\frac{L^{d}\hat{r}}{\lambda}\frac{\partial}{\partial t}\bar{\psi}_{X}(M,t) = \left\{\frac{\partial^{2}}{\partial M^{2}} + \frac{1}{2}H_{X}''(M) - \frac{1}{4}\left[H_{X}'(M)\right]^{2}\right\}\bar{\psi}_{X}(M,t) \quad (56)$$

After the change of variable

$$M = (L^{d}\hat{g})^{-1/4} q, \qquad \bar{\psi}_{X}(M, t) = \psi_{X}(q, t)$$
(57)

the Schrödinger equation becomes

$$-\frac{\hat{r}}{2\lambda} \left(\frac{L^d}{\hat{g}}\right)^{1/2} \frac{\partial}{\partial t} \psi_X(q,t) = h\left(\frac{1}{i}\frac{\partial}{\partial q},q\right) \psi_X(q,t)$$
(58)

with the Hamiltonian

$$h(p,q) = \frac{1}{2}p^2 + \frac{1}{2}q^2\left(\kappa + \frac{1}{12}q^2\right)^2 - \frac{1}{8}q^2 - \frac{\kappa}{2}$$
(59)

and

$$\kappa = \frac{1}{2} \left[\left(\frac{L^d}{\hat{g}} \right)^{1/2} \hat{\tau} + \left(\frac{\hat{f}}{\hat{g}} \right)^{1/2} X \right]$$
(60)

Given an initial wave function ψ_X at time t', the solution of Eq. (58) may be written in the form

$$\psi_{X}(q, t) = \int_{-\infty}^{\infty} dq' G(\kappa; q, t \mid q', t') \psi_{X}(q', t')$$
(61)

The expansion of the Green function $G(\kappa; q, t | q', t')$ in terms of eigenfunctions $\phi_{\kappa,n}(q)$ (with eigenvalues $\varepsilon_{\kappa,n}$) of the Hamiltonian is given by

$$G(\kappa; q, t \mid q', t') = \sum_{n} \phi_{\kappa,n}(q) \phi_{\kappa,n}(q')^* \exp\left[-\frac{2\lambda}{\hat{r}} \left(\frac{\hat{g}}{L^d}\right)^{1/2} \varepsilon_{\kappa,n}(t-t')\right]$$
(62)

In ref. 23, some exact eigenvalues $\varepsilon_{\kappa,n}$ for $n \leq 5$ are computed by a discretization technique. For each n = 2, 3, ... there is a lowest-lying eigenvalue $\varepsilon_n^{(\min)}$, where $0 < \varepsilon_2^{(\min)} < \varepsilon_3^{(\min)} < \cdots$. These eigenvalues accumulate in the region where $-\kappa$ is of order unity. For $n = 1, \varepsilon_{\kappa,1}$ is an increasing function of κ with $\lim_{\kappa \to -\infty} \varepsilon_{\kappa,1} = 0$. Thus the "energy bands" with small *n* govern the long-time behavior of the Green function.

The exact ground state $\phi_{\kappa,0}(q)$ with energy $\varepsilon_{\kappa,0} = 0$ corresponds via Eq. (55) to the equilibrium distribution $P_{\chi}^{\infty}(q)$, and the Green function is related to the transition probability by

$$P_{\chi}(q' \to q, t - t') = G(\kappa; q, t \mid q', t') \frac{\phi_{\kappa,0}(q)}{\phi_{\kappa,0}(q')}$$
(63)

Exploiting Eqs. (63) and (62), we obtain a representation of correlation functions in terms of quantum mechanical eigenfunctions:

$$\langle \mathscr{A}(q(t)) \mathscr{A}(q(t')) \rangle_{\chi}$$

$$= \langle \mathscr{A}(q) \rangle_{\chi}^{2} + \sum_{n \neq 0} |\langle \phi_{\kappa,n}| \mathscr{A}(q) |\phi_{\kappa,0}\rangle|^{2} e^{-|t-t'|/\tau_{k,n}}$$
(64)

Here $\langle \mathscr{A}(q) \rangle_{\chi} = \langle \phi_{\kappa,0} | \mathscr{A}(q) | \phi_{\kappa,0} \rangle$ is an equilibrium expectation value. The relaxation times²

$$\tau_{\kappa,n} = \frac{\hat{r}}{2\lambda} \left(\frac{L^d}{\hat{g}}\right)^{1/2} \frac{1}{\varepsilon_{\kappa,n}}$$
(65)

² Note that at the random fixed point $\tau_{\kappa,n}$ is of the order $\varepsilon^{-1/4}$. This is in agreement with the time rescaling given in Eq. (23).

as well as the functions $\phi_{\kappa,n}$ depend on the random variable X. Once the $\varepsilon_{\kappa,n}$ are known, we are able to transform the distribution of X to a distribution of relaxation times. The average of correlation functions with respect to disorder can be rewritten as

$$\overline{\langle \mathscr{A}(q(t)) \mathscr{A}(q(t')) \rangle} - \overline{\langle \mathscr{A}(q)^{2} \rangle} = \int_{0}^{\infty} \frac{d\theta}{(2\pi\sigma^{2})^{1/2}} \sum_{n \neq 0} |\gamma_{n}'(\theta)| \exp\left\{-\frac{1}{2\sigma^{2}} [\gamma_{n}(\theta) - \bar{\kappa}]^{2}\right\} \times |\langle \phi_{\gamma_{n}(\theta),n}| \mathscr{A}(q) |\phi_{\gamma_{n}(\theta),0} \rangle|^{2} \exp\left(-\frac{\lambda \hat{\tau}}{\hat{r}\bar{\kappa}} \frac{|t-t'|}{\theta}\right)$$
(66)

The function $\gamma_n(\theta)$ gives the value of the parameter κ such that $\varepsilon_{\kappa,n} = 1/\theta$. If $\varepsilon_{\kappa,n}$ as a function of κ is not one-to-one (this is the case for $n \ge 2$), we have to divide the region $-\infty < X < \infty$ into appropriate intervals in which $\gamma_n(\theta)$ is well defined. In Eq. (66), $\bar{\kappa}$ and the variance σ^2 are given by

$$\bar{\kappa} = \frac{1}{2} \left(\frac{L^d}{\hat{g}} \right)^{1/2} \hat{\tau}, \qquad \sigma^2 = \frac{\hat{f}}{4\hat{g}} \tag{67}$$

At the fixed point one obtains the scaling behavior

$$\bar{\kappa}(\tau, L) = \frac{1}{2} \left[\frac{(2\pi)^d G_{\varepsilon}}{u_*} \right]^{1/2} \frac{y T(y)}{[G(y)]^{1/2}}$$
(68)

$$\sigma(\tau, L)^{2} = \frac{v_{*}}{4u_{*}} \frac{F(y)}{G(y)}$$
(69)

with the functions F(y), G(y), and T(y) defined in (32).

The spectral density $\rho_{\mathcal{A}}$ is related to the normalized correlation function

$$\Phi_{\mathscr{A}}(t-t') = \frac{\overline{\langle \mathscr{A}(q(t)) \mathscr{A}(q(t')) \rangle} - \overline{\langle \mathscr{A}(q) \rangle^2}}{\overline{\langle \mathscr{A}(q)^2 \rangle} - \overline{\langle \mathscr{A}(q) \rangle^2}}$$
(70)

by

$$\Phi_{\mathscr{A}}(t-t') = \int_0^\infty d\tau \,\rho_{\mathscr{A}}(\tau) \,e^{-|t-t'|/\tau} \tag{71}$$

(Here the relaxation time τ should not be mixed up with the temperature parameter. In the sequel the scaled temperature variable y shall be used.) From Eq. (66) one easily derives the scaling behavior

$$\rho_{\mathscr{A}}(L, y; \tau) = L^{-z} \rho_{\mathscr{A}}(1, y; L^{-z} \tau)$$
(72)

At the bulk critical temperature $T = T_c$ (i.e., y = 0) we find in particular

$$\rho_{\mathcal{A}}(L,0;\tau) = 2\lambda\mu^2 \left(\frac{\mu L}{2\pi}\right)^{-z} A\rho_{0,\mathcal{A}}\left(2\lambda\mu^2\tau \left(\frac{\mu L}{2\pi}\right)^{-z}A\right)$$
(73)

with the scaling factor

$$A = \frac{1}{R(0)} \left[\frac{u_* G(0)}{(2\pi)^d G_c} \right]^{1/2}$$
(74)

and the universal scaling function

$$\rho_{0,\mathscr{A}}(\theta) = \frac{1}{c_{\mathscr{A}}(2\pi\sigma^2)^{1/2}} \sum_{n\neq 0} |\gamma'_n(\theta)| \exp\left\{-\frac{1}{2\sigma^2} \left[\gamma_n(\theta) - \bar{\kappa}\right]^2\right\}$$
$$\times |\langle \phi_{\gamma_n(\theta),n}| \mathscr{A}(q) |\phi_{\gamma_n(\theta),0} \rangle|^2 \tag{75}$$

At leading order in $\varepsilon^{1/4}$ we have at the critical point

$$\bar{\kappa} = \frac{1}{4} \left(\frac{3\varepsilon}{106} \right)^{1/4} \pi \sigma(0) (1 + O(\sqrt{\varepsilon})), \qquad \sigma^2 = \frac{1}{16} (1 + O(\varepsilon)) \tag{76}$$

The density $\rho_{\mathscr{A}}$ is normalized by the static correlation of \mathscr{A} , i.e.,

$$c_{\mathscr{A}} = \overline{\langle \mathscr{A}(q)^2 \rangle} - \overline{\langle \mathscr{A}(q) \rangle^2}$$
(77)

Notice that for a pure system (fixed point $v_* = 0$, $\sigma^2 = 0$) $\rho_{0, \mathscr{A}}$ becomes a sum of δ -functions reflecting a discrete spectrum of relaxation times.

According to Eq. (65), the largest relaxation times correspond to the lowest energy levels with a nonvanishing matrix element $\langle \phi_{\kappa,n} | \mathscr{A}(q) | \phi_{\kappa,0} \rangle$. In this paper, we consider as examples the odd quantity (with respect to parity) $\mathscr{A}(q) = q$ and $\mathscr{A}(q) = q^2$ as an even observable. While the behavior of $\rho_{\mathscr{A}}(\theta)$ is governed by the first exited state $\phi_{\kappa,1}$, the largest possible relaxation times of q^2 occur for n = 2. To obtain approximate results for eigenvalues as well as for eigenfunctions we start from the variational ansatz⁽²²⁾

$$\phi_{\kappa,1}(q) = N_1 q e^{-\alpha (q^2 + \beta)^2}$$
(78)

and

$$\phi_{\kappa,2}(q) = N_2(1 - Bq^2) e^{-\alpha(q^2 + \beta)^2}$$
(79)

Here $N_1(\alpha, \beta)$ and $N_2(\alpha, \beta)$ are normalization constants and the coefficient $B(\alpha, \beta)$ follows from orthogonality: $\langle \phi_{\kappa, 2} | \phi_{\kappa, 0} \rangle = 0$.

Oerding



Fig. 2. The relaxation time distribution $\rho_{q,0}$ of the order parameter. The broken line shows the asymptotic form described in the text.

The minima of

$$E_{\kappa,n}(\alpha,\beta) = \langle \phi_{\kappa,n} | h(p,q) | \phi_{\kappa,n} \rangle \qquad (n=1,2)$$
(80)

and the matrix elements $\langle \phi_{\kappa,n} | \mathscr{A}(q) | \phi_{\kappa,0} \rangle$ have been calculated for values of κ in the range $-0.5 < \kappa < 1.5$ (for n = 1) and $-1.5 < \kappa < 0.5$ (for n = 2) by the simplex method.⁽²⁴⁾ The results are used to interpolate the functions $\gamma_n(\theta)$ and $\langle \phi_{\gamma_n(\theta),n} | \mathscr{A}(q) | \phi_{\gamma_n(\theta),0} \rangle$ by means of the interpolation routine of Mathematica.⁽²⁵⁾ This procedure yields the scaling functions $\rho_{q,0}(\theta)$ and $\rho_{q^2,0}(\theta)$ shown in Figs. 2 and 3.

The singularity $\rho_{q^2,0}(\theta) \sim (\theta_m - \theta)^{-1/2}$ at $\theta_m \approx 1.69$ is due to a minimum of $\varepsilon_{k,2}$ and coincides with the largest relaxation time of q^2



Fig. 3. The relaxation time distribution $\rho_{q^2,0}$.

correlations. For $t \ge \theta_m$ (with a scaled time $t \propto L^{-z}t$) the correlation function $C_{q^2}(t)$ shows an exponential behavior

$$C_{a^2}(t) \sim e^{-t/\theta_m} \tag{81}$$

while for $i \approx \theta_m$ contributions of short relaxation times are appreciable and induce a faster decay. This behavior is expected for all even observables $\mathscr{A}(q)$.

A very different situation occurs for $\mathscr{A}(q) = q$. The long-time tail of $\rho_{q,0}(\theta)$ results from the almost degenerate ground state of the Hamiltonian h(p, q) in the limit $\kappa \to -\infty$. This effect may be explained physically by the local shift of the temperature caused by impurities: There are regions in the system where the temperature is shifted considerably below T_c and, as a mesoscopic analog of spontaneous symmetry breaking, parallel spin configurations decay very slowly.

While the variational method gives sufficiently accurate results for the region of θ displayed in Fig. 2, the asymptotic behavior of $\gamma_n(\theta)$ for $\theta \to \infty$ may be derived by instanton methods. The energy of the first exited state behaves as

$$\varepsilon_{\kappa,1} = \left(\frac{6}{\pi}\right)^{1/2} (-\kappa) \exp\left[-(6\kappa^2 + 3/2)\right] \quad \text{for} \quad \kappa \to -\infty$$
 (82)

A short derivation of this behavior is given in the appendix. Solving Eq. (82) for κ , we get

$$\gamma_1(\theta) \simeq -\left(\frac{1}{6}\ln\left(\frac{\theta}{\sqrt{\pi}}\right) + \frac{1}{12}\ln\ln\theta - \frac{1}{4}\right)^{1/2} \quad \text{for} \quad \theta \to \infty$$
 (83)

To obtain an approximation for the matrix element $\langle \phi_{\kappa,1} | q | \phi_{\kappa,0} \rangle$ we use the variational wave function (78) with $\alpha = 1/48$, $\beta = 12\kappa$ [this choice minimizes the energy $E_{\kappa,1}(\alpha, \beta)$ for $\kappa \to -\infty$]:

$$\langle \phi_{\kappa,1} | q | \phi_{\kappa,0} \rangle \simeq (-12\kappa)^{1/2} \quad \text{for} \quad \kappa \to -\infty$$
 (84)

This result is robust on changes of the variational wave function since any ansatz $\phi_{\kappa,1}(q) \propto q^n \exp[-(q^2 + 12\kappa)^2/48]$ with an odd exponent $n \ge 1$ gives the limiting behavior (84).

In Fig. 2 the asymptotic form of $\rho_{q,0}(\theta)$ is compared with the numerical result for $\theta \le 20$.

6. DISCUSSION

Finite-size scaling effects of the Ising model with random impurities have been investigated. Since the relaxation of this system is strongly affected by disorder, special attention was focused on dynamics. While the linear relaxation of a pure system may be described by a discrete set of relaxation times, impurities generate a continuous spectrum. We have calculated the spectral density for correlations of the magnetization M and for correlations of M^2 at the critical point. The results show that M^2 correlations decay exponentially for large scaled times $\tilde{t} = L^{-z}t$, whereas correlations of the magnetization display a power-like behavior.

The continuous spectrum of relaxation times, especially the arbitrarily long relaxation times of the magnetization, is a remarkable difference from the pure Ising model. It can be explained as follows. Since the impurities tend to hamper the formation of magnetic order, the critical temperature $T_c(p)$ of the random system is shifted below that of the pure system, $T_c(1)$. If the system is sufficiently large, there will be large regions almost free of impurities in which parallel spin configurations decay very slowly at temperatures below $T_c(1)$. In regions with a high concentration of impurities, on the other hand, the relaxation takes place very rapidly. Since the homogeneous mode of the magnetization contains contributions from different regions of the system with different concentrations of impurities and different relaxation rates, the spectrum becomes continuous in the finitesize scaling limit $(L \to \infty, \xi \to \infty, \xi/L \text{ arbitrary})$.

The long relaxation times of the order parameter have thus the same origin as the nonanalytic behavior above the critical temperature in dilute Ising magnets (Griffiths singularities).⁽²⁶⁾ In the thermodynamic limit there are arbitrarily large regions free of impurities in which the system tends to order below the critical point of the pure system. As a result the magnetization below $T_c(1)$ is a nonanalytic function of the external magnetic field. This is true even for concentrations of magnetic sites below the percolation threshold p_c .

Because of this relationship between relaxation times and Griffits singularities one might speculate that the long-time tail in the spectrum of M occurs at all temperatures below $T_c(1)$ and concentrations $p_c . But this is beyond the validity of the field-theoretic approach presented in this paper and should be checked by computer simulations. At least near the critical point of the random system the spectral densities of <math>M$ and M^2 retain their qualitative form.

The functions $\rho_{0,q}$ and ρ_{0,q^2} shown in Figs. 2 and 3 describe the spectral densities in the asymptotic scaling region at the critical point. For extreme concentrations (close to the percolation threshold or $p \leq 1$) a very large system size is required to observe the asymptotic scaling behavior. If, for example, the impurities are very dilute and the system is comparatively small ($L^3 = 50^3$, say) the spectrum is expected to be strongly peaked near the discrete relaxation times of the pure system. To calculate

nonasymptotic spectral densities by renormalization group techniques one has to study the flow of the coupling constants away from the fixed points. This leads to size-dependent effective coupling constants $\bar{u}(L)$ and $\bar{v}(L)$ and parameter functions $\hat{\tau}$, \hat{g} , f, and \hat{r} which violate the asymptotic scaling forms (32).

In a paper of Heuer⁽⁵⁾ the correlation function of |M| for a sitedisordered Ising system with a concentration p = 0.6 is shown. For this concentration the approach to the asymptotic region is quite slow. Crossover effects are expected to be less important for $p \approx 0.8$ since for this concentration even comparatively small systems may be described by asymptotic exponents.⁽⁴⁾

An interesting subject for further studies is the nonlinear relaxation of the magnetization at T_c . In the case of a pure system with an initial magnetization $M_0 \gg L^{-\beta/\nu}$ the relaxation displays a crossover from the bulk behavior $M(t) \sim t^{-\beta/(\nu z)}$ to an exponential decay.⁽²²⁾ This behavior will be changed in the presence of random impurities due to the continuous relaxation time spectrum of the order parameter.

If initial correlations are of short range, the magnetization grows at early times $t \ll M_0^{-\nu z/(\beta + \nu z \theta')}$ like a power $t^{\theta'}$ with a new exponent θ' .^(27,16) In connection with finite-size scaling this initial slip behavior is discussed in ref. 28.

APPENDIX

To obtain the energy $\varepsilon_{\kappa,1}$ of the first excited state of the Hamiltonian h(p, q) in the limit $\kappa \to -\infty$ we rescale the coordinate $q \to q' = q/\sqrt{-\kappa}$ and rewrite the stationary Schrödinger equation in the form

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial q^2} + \kappa^2 V\left(\frac{q}{-\kappa}\right)\right)\phi_{\kappa,1}(q) = \bar{\varepsilon}_{\kappa,1}\phi_{\kappa,1}(q) \tag{A1}$$

with

$$\bar{\varepsilon}_{\kappa,1} = \frac{1}{(-\kappa)} \varepsilon_{\kappa,1} - \frac{1}{2}$$
 (A2)

and the potential

$$V(q) = \frac{1}{2} q^2 \left(1 - \frac{q^2}{12} \right)^2 - \frac{1}{8\kappa^2} q^2$$
 (A3)

While the degeneracy between q = 0 and $q = \pm \sqrt{12}$ is lifted at first order in $1/\kappa^2$, the classical minima at $q = \pm \sqrt{12}$ correspond to quantum mechanical energy levels which are degenerate at all order in the perturbation theory.⁽¹¹⁾ We calculate the energy gap $\bar{\varepsilon}_{\kappa,1} - \bar{\varepsilon}_{\kappa,0}$ by an instanton method which is described in detail in ref. 29. Consider the quantity

$$\operatorname{Tr} P e^{-\beta H} = \sum_{n} (-1)^{n} e^{-\beta \hat{c}_{\kappa,n}}$$
(A4)

where P is the parity operator and H denotes the Hamiltonian on the l.h.s. of Eq. (A1). For $\kappa \to -\infty$, $\beta \to \infty$ the trace is dominated by

$$\operatorname{Tr} P e^{-\beta H} \simeq \beta(\bar{\varepsilon}_{\kappa,1} - \bar{\varepsilon}_{\kappa,0}) e^{-\beta \bar{\varepsilon}_{\kappa,0}}$$
(A5)

In the same limits we obtain by a quasiclassical approximation⁽²⁹⁾

Tr
$$Pe^{-\beta H} \simeq 2 \frac{(-\kappa)}{(2\pi)^{1/2}} \beta \left[\frac{\partial E(\beta)}{\partial \beta} \right]^{1/2} \exp[-\kappa^2 S(\beta)]$$
 (A6)

Here $E(\beta)$ and $S(\beta)$ are the energy and classical action of a particle moving in the potential -V(q) on a trajectory which connects the classical turning points $\pm q_i$ [i.e., $V(\pm q_i) + E = 0$]. β is the time required for one passage from $-q_i$ to q_i . Since this trajectory only exists for $V(\pm q_i) < V(0)$, we may not *a priori* neglect the term proportional to $1/\kappa^2$ in the potential (A3). For small $1/\kappa^2$ and $\beta \to \infty$ we obtain

$$q_{t} = \sqrt{12} \left[1 + \frac{1}{16\kappa^{2}} + O\left(\frac{1}{\kappa^{4}}\right) \right]$$
(A7)

$$E(\beta) = \frac{3}{2\kappa^2} + O\left(\frac{1}{\kappa^4}\right) - 6144\kappa^4 e^{-2\beta} \left[1 + O\left(\frac{\ln(-\kappa)}{\kappa^2}\right)\right]$$
(A8)

and

$$S(\beta) = \int_{-q_{t}}^{q_{t}} dq \left\{ 2\left[V(q) + E(\beta)\right] \right\}^{1/2} - E(\beta)\beta$$
$$= -\beta \frac{3}{2\kappa^{2}} \left[1 + O\left(\frac{1}{\kappa^{2}}\right) \right] + 6\left(1 + \frac{1}{4\kappa^{2}}\right)$$
$$+ \frac{3}{\kappa^{2}} \ln(-4\kappa) + O\left(\frac{\ln(-\kappa)}{\kappa^{4}}\right)$$
(A9)

Inserting these expressions into Eq. (A6) yields

Tr
$$Pe^{-\beta H} \simeq \left(\frac{6}{\pi}\right)^{1/2} \beta e^{\beta/2} e^{-(6\kappa^2 + 3/2)}$$
 (A10)

Thus the asymptotic form of the energy $\varepsilon_{\kappa,1}$ in the limit $\kappa \to -\infty$ is given by

$$\varepsilon_{\kappa,1} = \left(\frac{6}{\pi}\right)^{1/2} (-\kappa) e^{-(6\kappa^2 + 3/2)}$$
(A11)

ACKNOWLEDGMENTS

It is a pleasure to thank H. K. Janssen for interesting discussions and R. Blossey for a critical reading of the manuscript. This work has been supported by Sonderforschungsbereich 237 (Unordnung und grosse Fluktuationen) of the Deutsche Forschungsgemeinschaft.

REFERENCES

- I. O. Mayer, Critical exponents of the dilute Ising model from four-loop expansions, J. Phys. A 22:2815-2823 (1989).
- D. J. W. Geldart and K. De'Bell, Logarithmic corrections for dilute uniaxial ferromagnets at the critical dimension, J. Stat. Phys. 73:409-414 (1993).
- H.-O. Heuer, Monte Carlo simulation of strongly disordered Ising ferromagnets, *Phys. Rev. B* 42:6476-6484 (1990).
- H.-O. Heuer, Critical crossover phenomena in disordered Ising systems, J. Phys. A 26:L333-L339 (1993).
- 5. H.-O. Heuer, Dynamic scaling of disordered Ising systems, J. Phys. A 26:L341-L346 (1993).
- E. Sengespeick, Feldtheorie des kritischen Verhaltens von ungeordneten Ising-Systemen, Diploma thesis, Düsseldorf (1994); E. Sengespeick, H. K. Janssen, and K. Oerding, to be published.
- 7. M. E. Fisher, The theory of critical point singularities, in *Critical Phenomena*, M. S. Green, ed. (Academic Press, New York, 1971), pp. 1-99.
- E. Brézin, and J. Zinn-Justin, Finite size effects in phase transitions, Nucl. Phys. B 257[FS14]:867-893 (1985).
- 9. H. W. Diehl, Finite size effects in critical dynamics and the renormalization group, Z. Phys. B 66:211-218 (1987).
- Y. Y. Goldschmidt, Finite size scaling effects in dynamics, Nucl. Phys. B 280 [FS18]: 340-354 (1987).
- J. C. Niel and J. Zinn-Justin, Finite size effects in critical dynamics, Nucl. Phys. B 280[FS18]:355-384 (1987).
- H. K. Janssen, B. Schaub, and B. Schmittmann, Finite size scaling for directed percolation and related stochastic evolution process, Z. Phys. B 71:377-385 (1988).
- H. K. Janssen, B. Schaub, and B. Schmittmann, The general epidemic process in a finite environment, J. Phys. A 21:L427-L434 (1988).
- H. K. Janssen, On a Lagrangian for classical field dynamics and renormalization group calculations of dynamical properties, Z. Phys. B 23:377-380 (1976); C. De Dominicis, Techniques de renormalisation de la théorie des champs et dynamique des phénomènes critiques, J. Phys. (Paris) Coll. C1:247-253 (1976).

- C. De Dominicis and L. Peliti, Field-theory renormalization and critical dynamics above T_s: Helium, antiferromagnets, and liquid-gas systems, *Phys. Rev. B* 18:353-376 (1978).
- H. K. Janssen, On the renormalized field theory of nonlinear critical relaxation, in From Phase Transitions to Chaos, Topics in Modern Statistical Physics, G. Györgyi, I. Kondor, L. Sasvári, and T. Tél, eds. (World Scientific, Singapore, 1992), p. 68-91.
- A. B. Harris, Effect of random defects on the critical behavior of Ising models, J. Phys. C 7:1671-1692 (1974); A. B. Harris and T. C. Lubensky, Renormalization-group approach to the critical behavior of random-spin models, Phys. Rev. Lett. 33:1540-1543 (1974).
- 18. C. De Dominicis, Dynamics as a substitute for replicas in systems with quenched random impurities, *Phys. Rev. B* 18:4913-4919 (1978).
- I. D. Lawrie and V. V. Prudnikov, Static and dynamic properties of systems with extended defects: Two-loop approximation, J. Phys. C 17:1655-1668 (1984).
- 20. I. H. Sneddon, The Use of Integral Transforms (McGraw-Hill, New York, 1972).
- K. Binder, Finite size scaling analysis of Ising model block distribution functions, Z. Phys. B 43:119-140 (1981).
- 22. Y. Y. Goldschmidt, Dynamical relaxation in finite size system, Nucl. Phys. B 285[FS19]:519-534 (1987).
- 23. H. Dekker and N. G. van Kampen, Eigenvalues of a diffusion process with a critical point, *Phys. Lett. A* 73:374-376 (1979).
- 24. R. W. Daniels, An Introduction to Numerical Methods and Optimization Techniques (Elsevier North-Holland, New York, 1978).
- 25. S. Wolfram, Mathematica (Addison-Wesley, Redwood City, California, 1991).
- 26. R. B. Griffiths, Nonanalytic behavior above the critical point in a random Ising ferromagnet, *Phys. Rev. Lett.* 23:17-19 (1969); J. L. Cardy and A. J. McKane, Field theoretic approach to the study of Yang-Lee and Griffiths singularities in the randomly diluted Ising model, *Nucl. Phys. B* 257[FS14]:383-396 (1985).
- H. K. Janssen, B. Schaub, and B. Schmittmann, New universal short-time scaling behavior of critical relaxation processes, Z. Phys. B 73:539-549 (1989).
- H. W. Diehl and U. Ritschel, Dynamical relaxation and universal short-time behavior in finite systems, J. Stat. Phys. 73:1-20 (1993).
- 29. J. Zinn-Justin, The principles of instanton calculus, in Lectures at Les Houches Summer School, J.-B. Zuber and R. Stora, eds. (North-Holland, Amsterdam, 1984), p. 39.