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Universal finite-size scaling amplitudes in anisotropic scaling

Malte Henkel[1] **and Ulrich Schollwöck**[2]

[1] Laboratoire de Physique des Matériaux[3], Université Henri Poincaré Nancy I, BP 239, F–54506 Vandœuvre-les-Nancy Cedex, France
[2] Sektion Physik, Ludwig-Maximilians-Universität München, Theresienstr. 37/III, D–80333 München, Germany

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Abstract

Phenomenological scaling arguments suggest the existence of universal amplitudes in the finite-size scaling of certain correlation lengths in strongly anisotropic or dynamical phase transitions. For equilibrium systems, provided that translation invariance and hyperscaling are valid, the Privman–Fisher scaling form of isotropic equilibrium phase transitions is readily generalized. For non-equilibrium systems, universality is shown analytically for directed percolation and is tested numerically in the annihilation–coagulation model and in the pair contact process with diffusion. In these models, for both periodic and free boundary conditions, the universality of the finite-size scaling amplitude of the leading relaxation time is checked. Amplitude universality reveals strong transient effects along the active–inactive transition line in the pair contact process.

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1. Introduction

The notions of scaling and universality are central to the modern understanding of critical phenomena: see, for example, [1–3]. Besides the well known universality of the critical exponents, universality is also manifest for many critical amplitudes, as reviewed in [4]. Here we are concerned with universal amplitudes which arise in finite-size scaling. For example, consider a statistical system at equilibrium, such as a simple ferromagnet, which is described by an isotropic and translation-invariant field theory in its continuum limit. Close to its critical point, and on a lattice with finite extent L, Privman and Fisher [5] showed that in any dimension d below the upper critical dimension d^* the singular part of the free energy density f and the inverse of the correlation lengths ξ_i satisfy the scaling form

$$f(t,h) = L^{-d} Y(z_1, z_2) \qquad \xi_i^{-1} = L^{-1} S_i(z_1, z_2) \tag{1}$$

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where $z_1 = C_1 t L^{1/\nu}$, $z_2 = C_2 h L^{(\beta+\gamma)/\nu}$ are the scaling variables, the reduced temperature $t = (T - T_c)/T_c$ and the reduced magnetic field $h = H/T_c$ describe the distance from the critical point and β, γ, ν are the standard equilibrium critical exponents. The index i distinguishes different correlation lengths: for example, $i = \sigma$ for the spin–spin correlation length or $i = \varepsilon$ for the energy–energy correlation length in a simple ferromagnet. Furthermore, the scaling functions Y and S_i are *universal* functions and all non-universal properties of a given model are condensed in the values of the non-universal metric factors C_1 and C_2. Although the functions Y, S_i are universal, they do depend on the boundary conditions and on the geometric shape of the lattices under study.

It follows from (1) that if the model parameters are tuned to $t = h = 0$ so that the model is at its bulk critical point, the finite-size scaling of free energy density $f = L^{-d} Y(0, 0)$ and of the inverse correlation lengths $\xi_i^{-1} = L^{-1} S_i(0, 0)$ is described in terms of *universal* finite-size scaling amplitudes. This qualitative statement can be made quantitative in 2D for systems defined on an infinitely long strip of finite width L through a, by now, classic conformal invariance argument which, for example, explicitly relates the $S_i(0, 0)$ to known critical exponents [6]. Concrete model studies have confirmed this many times, as reviewed in [3, 4]. More recently, similar relations have been conjectured also in 3D from the results of numerical studies in toruslike [7, 8] and spherical geometries [9, 10].

When considering the situation of *dynamical* scaling, where time and space scale differently, the extra degree of freedom might appear to exclude the presence of universal finite-size scaling amplitudes in the sense of equation (1). Here, we shall ask under what conditions the arguments of Privman and Fisher [5] can be generalized also to anisotropic scaling—specifically, for a system undergoing a phase transition with anisotropic scaling which is defined on a lattice with finite extent L in the spatial direction but is infinite in the temporal direction. Then (under conditions to be detailed in sections 2 and 3) the *spatial* correlation lengths should satisfy the scaling form

$$\xi_{i,\perp}^{-1} = L^{-1} S_i\left(C_1 t L^{1/\nu_\perp}, C_2 h L^{(\beta+\gamma)/\nu_\perp}\right) \tag{2}$$

in a notation analogous to (1) and where, again, the S_i are universal functions.

While the generalization to *equilibrium* anisotropic scaling is a rather straightforward extension of the methods valid for the isotropic case [5], the non-equilibrium situation is more difficult. We shall show how correlation length amplitude universality can be established for systems in the directed percolation universality class. Furthermore, numerical data from some reaction–diffusion models are also in agreement with this and suggest that the scaling form (2) might be generally valid.

This paper is organized as follows. In section 2, we present the scaling arguments leading to the recognition of universal amplitudes for anisotropic scaling in equilibrium. In section 3 non-equilibrium dynamical scaling is discussed, with emphasis on the directed percolation universality class. In section 4, we test the amplitude universality by analysing the finite-size scaling of the leading inverse relaxation time in the annihilation–coagulation model and the pair contact process with single-particle diffusion. In section 5 we give our conclusions. The appendix contains the Bethe ansatz calculation of the relaxation time in an analytically solvable special case.

2. Universal finite-size amplitudes in equilibrium

Consider an equilibrium system with anisotropic scaling in two distinct directions. Systems of this kind have been known for a long time: for example, in Lifshitz points [11] or anisotropic uniaxial magnets [12] (see [13–16] for reviews) or else in quantum phase transitions [17]

(see [18] for a recent book). One can derive the phenomenological scaling of the physical observables from the covariance of the correlators under scale transformations and reconstruct the thermodynamics in this way [2,3]. In line with conventional phenomenological treatments of strongly anisotropic scaling [19,20], we assume for the two-point functions the scaling form

$$G_i\left(r_\perp, r_\parallel; t, h\right) = b^{-2x_i} G_i\left(\frac{r_\perp}{b}, \frac{r_\parallel}{b^\theta}; tb^{y_t}, hb^{y_h}\right) \tag{3}$$

where b is the rescaling factor, t, h refer to physical quantities like the reduced temperature and the reduced magnetic field, θ is the *anisotropy* exponent and y_t, y_h, x_i are scaling exponents. The index i refers to different physical quantities of which the two-point function is formed: for example, $i = \sigma$ for the spin operator or $i = \varepsilon$ for the energy density (for simplicity, we use throughout a notation analogous to simple ferromagnets). At criticality, $t = h = 0$, and one has

$$\begin{aligned} G_\sigma(r_\perp, 0) &\sim r_\perp^{-2x_\sigma} \qquad & G_\sigma(0, r_\parallel) &\sim r_\parallel^{-2x_\sigma/\theta} \\ G_\varepsilon(r_\perp, 0) &\sim r_\perp^{-2x_\varepsilon} \qquad & G_\varepsilon(0, r_\parallel) &\sim r_\parallel^{-2x_\varepsilon/\theta}. \end{aligned} \tag{4}$$

For a strongly anisotropic equilibrium system, $r_\perp$ and $r_\parallel$ correspond to different directions in space. This case is, for example, realized at the Lifshitz point in spin systems with competing interactions like the ANNNI model [15, 21]. For brevity, we refer to the directions $r_\perp$ as *'spatial'* and to the directions $r_\parallel$ as *'temporal'*.

We use the equilibrium fluctuation-dissipation theorem

$$\chi = \int \mathrm{d}r_\parallel \, \mathrm{d}^d r_\perp \, G_\sigma(r_\perp, r_\parallel) \qquad C = \int \mathrm{d}r_\parallel \, \mathrm{d}^d r_\perp \, G_\varepsilon(r_\perp, r_\parallel) \tag{5}$$

where d is the number of 'spatial' dimensions and χ, C are the susceptibility and specific heat. We shall work with a single 'temporal' direction throughout, but generalizations are obvious. Units are such that the critical temperature $T_\mathrm{c} = 1$. From (3) and integrating, one gets immediately the scaling forms for $\chi = \chi(t, h) = -\partial^2 f/\partial h^2$ and for $C = C(t, h) = -\partial^2 f/\partial t^2$. Here f is the (singular part) free energy density. From the scaling of χ and C, it should satisfy the scaling

$$f(t, h) = b^{\theta+d-2x_\sigma-2y_h} f(tb^{y_t}, hb^{y_h}) = b^{\theta+d-2x_\varepsilon-2y_t} f(tb^{y_t}, hb^{y_h}). \tag{6}$$

These two forms are consistent if $x_\sigma + y_h = x_\varepsilon + y_t = w$. In fact, the above argument works for any pair of scaling operators like σ, ε and their conjugated scaling fields h, t. Therefore, the value w must be independent of all physical scaling operators which might be present in a given model. Next, we define the standard static critical exponents α, β, γ as usual (see, for example, [2]). Also, out of criticality, we expect an exponential decrease of the two-point function, characterized by the correlation lengths $\xi_{\perp,\parallel} \sim t^{-\nu_{\perp,\parallel}}$ (at $h = 0$). From this, we find that $\nu_\perp = 1/y_t$, $\theta = \nu_\parallel/\nu_\perp$ and $\beta + \gamma = y_h/y_t$. From dimensional counting, we expect $w = d + \theta$ and the free energy density then scales as

$$f(t, h) = b^{-d-\theta} f(tb^{y_t}, hb^{y_h}). \tag{7}$$

As usual, we explicitly assume the absence of dangerously irrelevant scaling fields [1, 5, 19]. We then recover the *hyperscaling* relation $2 - \alpha = \nu_\parallel + d\nu_\perp$. The common scaling form for the thermodynamics is found by scaling out b and introducing the conventional critical exponents

$$f(t, h) = A_1 |t|^{2-\alpha} W^\pm\left(A_2 h |t|^{-\beta-\gamma}\right) \tag{8}$$

where $W^\pm$ are the universal scaling functions which are obtained for $t > 0$ and $t < 0$, respectively, and $A_{1,2}$ are non-universal metric constants. At this level, the anisotropy of the scaling of the two-point function only appears in the generalized form of the hyperscaling relation.

Equation (8) will be the starting point for our discussion of finite-size scaling. In what follows, we consider a situation where the 'spatial' directions are of finite extent L whereas the 'temporal' direction remains infinite. In the same spirit as Privman and Fisher [5], we assume that the *finite-size* scaling behaviour is governed by the 'spatial' correlation length $\xi_\perp$ only and we write

$$f(t,h;L) = A_1|t|^{2-\alpha} W^{\pm}\left(A_2 h|t|^{-\beta-\gamma}; L\xi_\perp^{-1}\right) \tag{9}$$

where the *bulk* 'spatial' correlation length $\xi_\perp = \xi_0 t^{-\nu_\perp}$. Note that there is *no* extra metric factor in the second argument of $W^{\pm}$, whereas ξ_0 is non-universal. To simplify the notation, we assume that there is no phase transition for L finite, but this restriction could be removed analogously to the equilibrium case [22]. We emphasize that the 'temporal' direction remains infinite, otherwise we would have to deal with two *distinct* finite length scales.

Following the ideas developed by Privman and Fisher [5], we have to trace the non-universal constants, taking into account the anisotropic scaling. For that, it is sufficient to study the 'spatially' infinite system. We expect the scaling form of the connected spin–spin correlator, see also (3),

$$G_\sigma(r_\perp, r_\parallel; t, h) = D_0 D_1 r_\perp^{-2x_\sigma} X^{\pm}\left(r_\perp/\xi_\perp, D_0 r_\parallel/\xi_\perp^{\theta}; D_2 h|t|^{-\beta-\gamma}\right) \tag{10}$$

where $X^{\pm}$ is a universal scaling function and $D_{0,1,2}$ are non-universal metric factors. From the fluctuation-dissipation theorem (5) one has

$$\chi(t,h) = D_1 \xi_\perp^{\gamma/\nu_\perp} \tilde{X}^{\pm}\left(D_2 h|t|^{-\beta-\gamma}\right). \tag{11}$$

where $\tilde{X}^{\pm}$ is a new scaling function obtained from $X^{\pm}$. Now, for the *non-connected* spin–spin correlator, one has in the same way, introducing new universal scaling functions $Z^{\pm}$

$$\Gamma_\sigma(r_\perp, r_\parallel; t, h) = D_0 D_1 r_\perp^{-2x_\sigma} Z^{\pm}\left(r_\perp/\xi_\perp, D_0 r_\parallel/\xi_\perp^{\theta}; D_2 h|t|^{-\beta-\gamma}\right). \tag{12}$$

At this point, we assume translation invariance with respect to $r_\perp$ and $r_\parallel$. Therefore, there should exist a mean magnetization m which is independent of $r_\perp$ and $r_\parallel$ and which can be found considering Γ_σ at large separations $r_\perp, r_\parallel$:

$$\Gamma_\sigma(r_\perp, r_\parallel; t, h) = D_0 D_1 \xi_\perp^{-2x_\sigma} Z^{\pm}\left(1, D_0 r_\parallel/r_\perp^{\theta}; D_2 h|t|^{-\beta-\gamma}\right) \tag{13}$$

$$\downarrow \qquad\qquad \downarrow$$

$$m^2(t,h) = D_0 D_1 \xi_\perp^{-2x_\sigma} \tilde{Z}^{\pm}\left(D_2 h|t|^{-\beta-\gamma}\right) \tag{14}$$

where the arrow indicates taking the limit of large 'spatio-temporal' separations. Because of translation invariance, m^2 should become independent of D_0. On the other hand, applying standard thermodynamics to the free energy (8) yields

$$m(t,h) = A_1 A_2 |t|^{\beta} W_1^{\pm}\left(A_2 h|t|^{-\beta-\gamma}\right) \tag{15}$$

$$\chi(t,h) = A_1 A_2^2 |t|^{-\gamma} W_2^{\pm}\left(A_2 h|t|^{-\beta-\gamma}\right) \tag{16}$$

where $W_n^{\pm}(x) = \mathrm{d}^n W^{\pm}(x)/\mathrm{d}x^n$.

We now compare equations (11) and (16). Letting first $h = 0$, we find

$$D_1 \xi_0^{\gamma/\nu_\perp} = A_1 A_2^2 U_1. \tag{17}$$

Comparing the arguments of the scaling functions, we have

$$D_2 = A_2 U_2. \tag{18}$$

Next, we compare equations (14) and (15) and find for $h = 0$ that

$$D_0 D_1 \xi_0^{-2\beta/\nu_\perp} = A_1^2 A_2^2 U_3 \tag{19}$$

(since $x_\sigma = \beta/\nu_\perp$). Here, $U_{1,2,3}$ are *universal* constants whose universality follows from the universality of the scaling functions considered. Using the hyperscaling relation $\gamma + 2\beta = (d+\theta)\nu_\perp$, we find that

$$\begin{aligned} A_1 \xi_0^{d+\theta} D_0^{-1} &= Q_1 = U_1/U_3 \\ D_2 A_2^{-1} &= Q_2 = U_2 \\ D_0^{\gamma/(\nu_\perp(d+\theta))} D_1 A_1^{-1-\gamma/(\nu_\perp(d+\theta))} A_2^{-2} &= Q_3 = U_1^{1-\gamma/(\nu_\perp(d+\theta))} U_3^{\gamma/(\nu_\perp(d+\theta))} \end{aligned} \tag{20}$$

and the $Q_{1,2,3}$ are universal constants.

Finally, we come back to the finite-size scaling behaviour. In equation (9), we replace ξ_0 by A_1 using (20). Scaling out L and using again hyperscaling, it is easy to arrive at the scaling form

$$f(t,h;L) = L^{-d-\theta} D_0 Y\big(C_1 t L^{1/\nu_\perp}, C_2 h L^{(\beta+\gamma)/\nu_\perp}\big) \tag{21}$$

where Y is a universal scaling function and $C_{1,2}$ are non-universal metric factors related to $A_{1,2}$. In contrast with the isotropic situation (1), we see that the finite-size scaling amplitude of the free energy is no longer universal. Furthermore, since $\xi_\parallel = \xi_\perp^\theta / D_0$, we have

$$f(t,0;L)\xi_\perp^d(t,0;L)\xi_\parallel(t,0;L) = D_0^{-1} f(t,0;L)\xi_\perp^{d+\theta}(t,0;L) \underset{t\to 0}{\to} \text{univ. constant} \tag{22}$$

which holds because of (20). Therefore, we expect for the *'spatial'* correlation length

$$\xi_\perp^{-1} = L^{-1} S\big(C_1 t L^{1/\nu_\perp}, C_2 h L^{(\beta+\gamma)/\nu_\perp}\big) \tag{23}$$

with a *universal* scaling function S and the *same* metric factors $C_{1,2}$ as in (21). While this analysis was phrased in terms of the transverse spin–spin correlation length $\xi_\perp = \xi_{\perp,\sigma}$, similar arguments should hold for the 'spatial' correlation lengths $\xi_{\perp,i}$ of any other physical observable, with S in (23) being replaced by an appropriate function S_i. The scaling functions Y and S_i should depend on the boundary conditions and, if $d \geqslant 2$, on the shape of the finite 'spatial' domain. Note that L refers here to the physical length, which cannot be equated to the number of sites N times the lattice constant in non-square lattices [5, 22]. For a recent example of this in the 2D Ising model context, see [23].

Finally, the 'temporal' correlation lengths $\xi_{\parallel,i}$ should read

$$\xi_{\parallel,i}^{-1} = L^{-\theta} D_0 R_i\big(C_1 t L^{1/\nu_\perp}, C_2 h L^{(\beta+\gamma)/\nu_\perp}\big) \tag{24}$$

with universal scaling functions R_i and again the *same* metric factors $C_{1,2}$ as before. The value of D_0 is related to the dimensionful constant which occurs in the energy–momentum dispersion relation of the underlying continuum field theory and cannot be found straightforwardly. However, at criticality ($t = h = 0$), ratios of 'temporal' correlation lengths $\xi_{\parallel,i}/\xi_{\parallel,j}$ should tend to universal constants in the $L \to \infty$ limit. The universality of these ratios would not have immediately been obvious from straightforward finite-size scaling.

Equation (23) is the main result of this section. It provides the natural generalization of the Privman–Fisher form (1) to the case of equilibrium anisotropic scaling. It is immediate to include further physical parameters into the analysis. We emphasize that (i) translation invariance and (ii) hyperscaling was required in deriving this result. We stress that we considered finite sizes in the 'spatial' direction and obtain universality for the spatial correlation lengths $\xi_{\perp,i}$ only.

3. Universal finite-size amplitudes out of equilibrium

We have seen that in equilibrium systems with anisotropic scaling and in a geometry where the 'spatial' directions are of finite extent L while the 'temporal' direction is infinite, the 'spatial'

correlation lengths have a universal finite-size scaling amplitude. We now ask whether this result generalizes towards more general forms of dynamical scaling, without appealing to the special properties of equilibrium systems. Fluctuations in non-equilibrium systems can be treated in terms of dynamic functionals via Martin–Siggia–Rose theory [24–27]. To be specific, we shall work in a setting of reaction–diffusion processes, of which directed percolation is a common example: see [28–31] for reviews. We shall continue to denote time by $r_\parallel$ and space by $r_\perp$. As before, t measures the distance from the steady-state critical point and h denotes an external field (for example, for directed percolation $t = p - p_c$ and h is the rate of a process $\emptyset \to A$). For the sake of technical simplicity, we shall assume translation invariance throughout. As in equilibrium, we have to trace the non-universal metric factors and this is most conveniently done in the bulk.

Physical quantities of interest are the mean particle density ρ, the survival probability P and the pair connectedness function $G = G(r'_\perp, r'_\parallel; r_\perp, r_\parallel)$, which is defined as the probability that the sites $(r'_\perp, r'_\parallel)$ and $(r_\perp, r_\parallel)$ are connected by a direct path [29,30]. Because of translation invariance $G = G(r'_\perp - r_\perp, r'_\parallel - r_\parallel)$, which will be used throughout. These quantities are expected to satisfy the scaling behaviour

$$\begin{aligned}
\rho(r_\perp, r_\parallel; t, h) &= b^{-x_\rho}\rho\left(\frac{r_\perp}{b}, \frac{r_\parallel}{b^z}; tb^{y_t}, hb^{y_h}\right) = D_{1\rho}\,\xi_\perp^{-x_\rho}\mathcal{E}^\pm\left(\frac{r_\perp}{\xi_\perp}, D_0\frac{r_\parallel}{\xi_\perp^z}; D_2 h|t|^{-y_h/y_t}\right)\\
P(r_\perp, r_\parallel; t, h) &= b^{-x_P}P\left(\frac{r_\perp}{b}, \frac{r_\parallel}{b^z}; tb^{y_t}, hb^{y_h}\right) = D_{1P}\,\xi_\perp^{-x_P}\mathcal{F}^\pm\left(\frac{r_\perp}{\xi_\perp}, D_0\frac{r_\parallel}{\xi_\perp^z}; D_2 h|t|^{-y_h/y_t}\right)\\
G(r_\perp, r_\parallel; t, h) &= b^{-x_G}G\left(\frac{r_\perp}{b}, \frac{r_\parallel}{b^z}; tb^{y_t}, hb^{y_h}\right) = D_{1G}\,\xi_\perp^{-x_G}\mathcal{G}^\pm\left(\frac{r_\perp}{\xi_\perp}, D_0\frac{r_\parallel}{\xi_\perp^z}; D_2 h|t|^{-y_h/y_t}\right)
\end{aligned} \tag{25}$$

where the x are scaling dimensions and $y_{t,h}$ renormalization group eigenvalues, the D are non-universal metric factors, $\mathcal{E}, \mathcal{F}, \mathcal{G}$ are universal scaling functions where the index distinguishes between the cases $t > 0$ and $t < 0$, $\xi_\perp = \xi_0|t|^{-\nu_\perp}$ is the spatial, $\xi_\parallel = \xi_\perp^z/D_0$ is the temporal correlation length and z is the dynamical exponent (as before, $y_t = 1/\nu_\perp$).

In the steady state, and for $h = 0$, one expects $\rho \sim t^\beta$ and $P \sim t^{\beta'}$. In general, the two exponents β and β' are distinct from each other. For spatial translation invariance, the dependence on $r_\perp$ drops out for both ρ and P and in the steady state (i.e. $r_\parallel \to \infty$) one has

$$\begin{aligned}
\rho(t, h) &= D_{1\rho}\,\xi_0^{-\beta/\nu_\perp}\tilde{\mathcal{E}}^\pm\left(D_2 h|t|^{-y_h/y_t}\right)|t|^\beta\\
P(t, h) &= D_{1P}\,\xi_0^{-\beta'/\nu_\perp}\tilde{\mathcal{F}}^\pm\left(D_2 h|t|^{-y_h/y_t}\right)|t|^{\beta'}
\end{aligned} \tag{26}$$

where $x_\rho = \beta/\nu_\perp$, $x_P = \beta'/\nu_\perp$ and $\tilde{\mathcal{E}}^\pm = \lim_{r_\parallel\to\infty}\mathcal{E}^\pm$ and similarly for $\mathcal{F}$. We also consider the auto-connectedness (that is $r_\perp = r'_\perp$) in the steady state

$$G(0, \infty; t, h) =: G(t, h) = D_{1P}\,\xi_0^{-x_G}\tilde{\mathcal{G}}^\pm\left(D_2 h|t|^{-y_h/y_t}\right)|t|^{x_G\nu_\perp}. \tag{27}$$

In the active phase ($t > 0$), the surviving clusters will create an average density $\sim|t|^\beta$ in the interior of the spreading cone. Therefore, the auto-connectedness should in the steady state saturate at the value [32]

$$G(t, h) = \rho(t, h)P(t, h). \tag{28}$$

Comparison of the scaling forms then yields, setting $h = 0$,

$$x_G = (\beta + \beta')/\nu_\perp \qquad D_{1G} = D_{1\rho}D_{1P}\,\frac{\tilde{\mathcal{E}}^\pm(0)\tilde{\mathcal{F}}^\pm(0)}{\tilde{\mathcal{G}}^\pm(0)}. \tag{29}$$

Usually, $x_G = d - \theta z$ is expressed in terms of the initial critical slip exponent θ [33], which makes it apparent that expression (29) is in fact a generalized hyperscaling relation [29,30,32].

Next, we consider the total mass M of the cluster [30], given by

$$M(t,h) := \int_{\mathbb{R}^d} \mathrm{d}^d r_\perp \int_0^\infty \mathrm{d}r_\parallel \, G(r_\perp, r_\parallel; t, h) = \frac{D_{1G}}{D_0} \xi_\perp^{\gamma/\nu_\perp} \overline{\mathcal{G}}^{\pm} \left(D_2 h |t|^{-y_h/y_t} \right) \tag{30}$$

where equation (25) was used and $\overline{\mathcal{G}}^{\pm}$ is a new universal function related to $\mathcal{G}^{\pm}$. Also

$$\gamma = \mathrm{d}\nu_\perp + \nu_\parallel - \beta - \beta' \tag{31}$$

which is the analogue of the hyperscaling relation of the equilibrium systems.

While the discussion so far has been completely general, we now appeal to two properties which are valid for systems in the directed percolation universality class, but need not be generically valid. First, we consider a directed percolation process in the presence of a weak field h (physically, h parametrizes the rate of a particle creation process $\emptyset \to A$). A site at a given time becomes active if it is connected with at least one active site in the past, where a particle was created by the field. The number of such sites is equal to the cluster size; the probability to become active is given by the density [30]

$$\rho(t,h) \simeq 1 - (1-h)^{M(t,h)} \simeq hM(t,h) \tag{32}$$

for h small. Therefore,

$$M(t,0) = \left. \frac{\partial \rho(t,h)}{\partial h} \right|_{h=0}. \tag{33}$$

Comparison with the scaling forms for ρ and M leads to

$$y_h/y_t = \beta + \gamma \qquad D_{1P} = D_0 D_2 \xi_0^{-(\beta+\gamma)/\nu_\perp} \mathcal{A}^{\pm} \tag{34}$$

where $\mathcal{A}^{\pm}$ is an universal amplitude. Second, directed percolation is special in the sense that there is a 'duality' symmetry which can be used to show that [34]

$$\rho(t,h) = P(t,h). \tag{35}$$

As a consequence, $\beta = \beta'$ and $D_{1\rho} = D_{1P}$ for directed percolation and we thus have, combining equations (26), (30), (34),

$$\begin{aligned} \rho(t,h) &= D_0 D_2 \xi_0^{-d-z} |t|^{\beta} \hat{\mathcal{M}}_1^{\pm} \left(D_2 h |t|^{-\beta-\gamma} \right) \\ M(t,h) &= D_0 D_2^2 \xi_0^{-d-z} |t|^{-\gamma} \hat{\mathcal{M}}_2^{\pm} \left(D_2 h |t|^{-\beta-\gamma} \right) \end{aligned} \tag{36}$$

with universal functions $\hat{\mathcal{M}}_n^{\pm}(x) = \mathrm{d}^n \hat{\mathcal{M}}^{\pm}(x)/\mathrm{d}x^n$ and where the hyperscaling relation equation (31) has been used. We therefore recover the analogues of equations (15), (16) found in equilibrium. Finally, we define a new function $\mu = \mu(t,h)$ by $\rho(t,h) = \partial \mu(t,h)/\partial h$, which implies

$$\mu(t,h) = D_0 \xi_0^{-d-z} |t|^{(d+z)\nu_\perp} \hat{\mathcal{M}}^{\pm} \left(D_2 h |t|^{-\beta-\gamma} \right). \tag{37}$$

In particular, as we did before at equilibrium, we have because of $\xi_\parallel = \xi_\perp^z / D_0$ that

$$\mu(t,0) \xi_\perp^d(t,0) \xi_\parallel(t,0) \underset{t \to 0}{\to} \text{univ. constant} \tag{38}$$

which is indeed the analogue of the result (22).

Lastly, we consider a geometry of finite size L in space but of infinite extent in time. Again, by analogy with section 2, we postulate that in this finite geometry merely the scaling functions are modified

$$\hat{\mathcal{M}}_n^{\pm} = \hat{\mathcal{M}}_n^{\pm} \left(D_2 h |t|^{-\beta-\gamma}; L\xi_\perp^{-1} \right) \tag{39}$$

and without introducing any further metric factor. Indeed, we can then scale out L and, because of equation (38), arrive at the same scaling forms (23), (24) as had been found before

for the spatial and temporal correlation lengths in anisotropic equilibrium systems, at least for systems in the directed percolation universality class. Since directed percolation is known to be equivalent to an equilibrium (in fact, purely geometrical) problem, the existence of universal finite-size amplitudes in this class is not too surprising and might have been anticipated from the discussion in the previous section.

While the spatial correlation length $\xi_\perp$ may not be always a very accessible quantity, its universality may also be tested by considering the spatial moment (let $t = h = 0$ for simplicity)

$$\begin{aligned} R_L^{(n)} := \langle r_\perp^n \rangle &= \frac{\int_{\Lambda(L)} \mathrm{d}^d r_\perp \int_0^\infty \mathrm{d}r_\parallel \, r_\perp^n G(r_\perp, r_\parallel; L/\xi_\perp)}{\int_{\Lambda(L)} \mathrm{d}^d r_\perp \int_0^\infty \mathrm{d}r_\parallel \, G(r_\perp, r_\parallel; L/\xi_\perp)} \\ &= \xi_\perp^n \frac{\int_{\Lambda(L/\xi_\perp)} \mathrm{d}^d r_\perp \int_0^\infty \mathrm{d}r_\parallel \, r_\perp^{n-x_G} \mathcal{G}^\pm(r_\perp, r_\parallel; L/\xi_\perp)}{\int_{\Lambda(L/\xi_\perp)} \mathrm{d}^d r_\perp \int_0^\infty \mathrm{d}r_\parallel \, r_\perp^{-x_G} \mathcal{G}^\pm(r_\perp, r_\parallel; L/\xi_\perp)} \\ &= \xi_\perp^n \, \Xi_n(L/\xi_\perp) \\ &= L^n \, \tilde{\Xi}_n(L/\xi_\perp) \end{aligned} \tag{40}$$

where $\Lambda(L)$ is a d-dimensional hypercube of linear extent L and Ξ_n and $\tilde{\Xi}_n$ are universal functions. Since there is no metric factor in the argument of $\tilde{\Xi}_n$, the universality of the finite-size scaling amplitude of $\xi_\perp$ is equivalent to the universality of the finite-size scaling amplitude of $R_L^{(n)}$ (on the other hand, the temporal moment $\langle r_\parallel^n \rangle \sim (D_0^{-1} L^z)^n$ has a non-universal amplitude). The universality of these moments is a somewhat stronger statement than the universality of certain ratios of moments $\langle \rho^n \rangle$ of the particle density ρ which has recently been verified in 1D and in 2D for several models in the directed percolation universality class [35].

In summary, we have seen that for systems in the directed percolation universality class, the special properties equations (33), (35), taken together with the general relation (28), are sufficent to rederive the universal finite-size scaling form (23) of the spatial correlation length, in spite of the absence of the fluctuation-dissipation relation. It is not yet clear whether there exist more general arguments which would permit us to arrive at the same result without appealing to either (33) or (35). However, we shall in the next section present numerical evidence that the universal finite-size scaling forms (23) for $\xi_\perp$ or (24) for $\xi_\parallel$ might be more generally valid.

4. Reaction–diffusion processes

The new information contained in (23) which goes beyond the standard renormalization group ideas is the universality of the finite-size scaling amplitude $L\xi_\perp^{-1}$ precisely at criticality (and similarly the universality of *all* ratios $\xi_{\parallel,i}/\xi_{\parallel,j}$). Since, for the time being, the derivation of this universality for non-equilibrium systems appears to be restricted to directed percolation, we use the pair contact process and the annihilation–coagulation model to test the universality hypothesis advanced in sections 2 and 3 quantitatively.

The pair contact process [36] has been intensively studied recently. It is a reaction–diffusion system, where particles move and react on a lattice. While each lattice site can be either empty or be occupied by a single particle, the following microscopic moves are permitted (referred to as PCPD):

$$\begin{array}{lll} \left\{ \begin{array}{rcl} AA\emptyset & \to & AAA \\ \emptyset AA & \to & AAA \end{array} \right. & \text{with rate} & \dfrac{(1-p)(1-d)}{2} \\ AA \to \emptyset\emptyset & \text{with rate} & p(1-d) \\ A\emptyset \leftrightarrow \emptyset A & \text{with rate} & d \end{array} \tag{41}$$

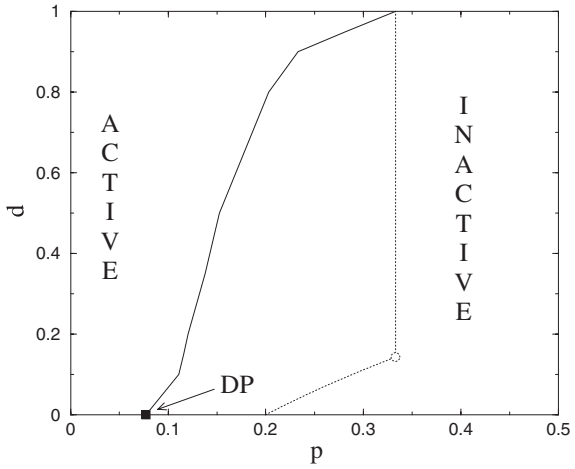

Figure 1. Steady-state phase diagram of the pair contact process. The dotted lines are the phase boundaries according to pair mean-field theory, while the full curve gives the active–inactive transition in 1D. DP marks the steady-state transition in the directed percolation universality class at $d = 0$.

and are parametrized by the diffusion constant d and the pair annihilation rate p.

While in the case without diffusion ($d = 0$), the steady-state transition between the active and the absorbing state was found to be in the directed percolation universality class [35–37], the effects of adding diffusion were first studied using field-theoretical methods, considering a bosonic field theory without any restriction on the number of particles per site (which leads to a divergent particle density in the active phase) [38]. It was shown that the entire absorbing phase is critical and in the universality class of diffusion–annihilation (see below). Because of the non-renormalizability of the underlying field theory, no quantitative information about the transition towards the active state could be obtained. The first quantitative information was obtained [39] through the use of density matrix renormalization group (DMRG) techniques [40–42]. The steady-state phase diagram is shown in figure 1 and there is a general agreement between DMRG and Monte Carlo studies on the location of the critical point $p_c(d)$ [39, 43–46].

The annihilation–coagulation model is formulated in the same way, with the allowed reactions

$$\begin{aligned} AA &\to A\emptyset,\ \emptyset A \quad \text{with rate } d\gamma \\ AA &\to \emptyset\emptyset \quad \text{with rate } 2d\alpha \\ A\emptyset &\leftrightarrow \emptyset A \quad \text{with rate } d \end{aligned} \tag{42}$$

parametrized by α and γ for annihilation and coagulation, respectively. The long-time behaviour of the model is always algebraic, i.e. the mean particle density $\rho(t) \sim t^{-1/2}$ in 1D: see [28–31, 47] and references therein.

In this paper, we use the Hamiltonian formulation of reaction–diffusion processes [48–52], which starts from the master equation

$$\frac{\partial |P(t)\rangle}{\partial t} = -H|P(t)\rangle \tag{43}$$

where $|P(t)\rangle$ a state vector and H is referred to as 'quantum' Hamiltonian (for recent reviews, see [30, 47]). For a chain with L sites, H is a stochastic $2^L \times 2^L$ matrix with elements

$$\langle\sigma|H|\tau\rangle = -w(\tau \to \sigma) \qquad \langle\sigma|H|\sigma\rangle = \sum_{\tau\neq\sigma} w(\sigma \to \tau) \tag{44}$$

where $|\sigma\rangle$, $|\tau\rangle$ are the state vectors of the particle configurations σ and τ, with w the transition rate. It is well known that the ground state energy of the pair contact process $E_0 = E_1 = 0$ is twofold degenerate for $d \neq 0$ [39]. The energy gap $\Gamma = E_2 - E_0$, calculated from the second excited state, is the inverse relaxation time or, in the notation of section 2, the inverse 'temporal' correlation length $\xi_\parallel^{-1} = \Gamma$ towards the steady state. We shall consider both free and periodic boundary conditions.

(1) First, we discuss the pair contact process (41). We find the following, surprisingly simple, finite-size scaling behaviour for the gap Γ_L *in the entire absorbing phase*, that is, for all $p \geqslant p_c(d)$, namely

$$\Gamma_L = adL^{-2}\big(1 + \mathrm{O}\big(L^{-1}\big)\big) \tag{45}$$

where a depends on the boundary condition

$$a = \begin{cases} 2\pi^2 & \text{periodic} \\ \pi^2 & \text{free} \end{cases} \tag{46}$$

but is *independent* of both p and d.

Before deriving (46), we argue that this result confirms the universality of the correlation length amplitudes discussed in section 3. Indeed, for systems in the diffusion–annihilation universality class already the inverse 'temporal' correlation length Γ has a universal amplitude, provided that the value of the diffusion constant d is fixed. The universality of the reaction–diffusion process $2A \to \emptyset$ has been discussed using field theory methods [53–55]. From the renormalization group equations, it can be shown that the value of the diffusion constant d is not renormalized through the effects of the interaction of the particles and simply stays at its bare value. The bare value of d is the value it has in the original lattice formulation of the problem. Since the diffusion constant sets the time scale, we expect for the gap $\Gamma \sim L^{-2}d$. These calculations [53–55] apply to the process $2A \to \emptyset$ which corresponds to the case $p = 1$ in the model at hand. However, it is known that in the entire absorbing phase, the extra interactions coming from the reaction $2A \to 3A$ are irrelevant [38]. Therefore, they should not modify the value of d (since we only consider here the inactive phase, we leave aside the question of how d evolves under renormalization in the active phase). Consequently, the proportionality of Γ and d in equation (45) comes from the non-renormalization of d. That non-renormalization is a special property of the diffusion–annihilation universality class. That is consistent with the scaling form (24) for $\xi_\parallel$ and we can identify $D_0 = d$. Finally, the p-independence of the amplitude a in equation (46) is an example of the universality of the finite-size scaling amplitude $R(0, 0)$ in equation (24), which in turn implies the universality of $S(0, 0)$ in equation (23).

We now derive equations (45), (46). We need the lowest non-vanishing eigenvalue $\Gamma = E_2$ of the quantum Hamiltonian H. For $p = 1$, it turns out that the spectrum of H is equal to the spectrum of an XXZ Heisenberg quantum chain H_{XXZ}. The lowest gap of H_{XXZ} can be found from the coordinate Bethe ansatz [56, 57]. This reproduces equation (46) for $p = 1$ and all values of d. The details of the calculation are presented in the appendix.

We point out, however, that for $d = 1/2$ and free boundary conditions only, the Bethe ansatz equations have a closed-form solution. The *exact* lowest gap for any finite number of sites L is

$$\Gamma_L = 1 - \cos\frac{\pi}{L+1} \qquad d = \tfrac{1}{2} \qquad p = 1 \qquad \text{free b.c.} \tag{47}$$

in agreement with (45), (46). This had been conjectured before on the basis of numerical data [42] (closed-form solutions for slightly different $\Delta = 1/2$ XXZ chains have been discussed recently in [58]).

For $p \neq 1$, the PCPD is not related to any known integrable model and we revert to numerical methods. We consider the normalized amplitudes

$$A_L^{(\mathrm{P})} = L^2\Gamma_L/(2\pi^2 d) \qquad A_L^{(\mathrm{F})} = L^2\Gamma_L/(\pi^2 d) \tag{48}$$

defined for periodic (P) and free (F) boundary conditions, respectively. If and only if (46) is correct, the amplitudes $A_L^{(\mathrm{P})}$ and $A_L^{(\mathrm{F})}$ should converge towards unity in the $L \to \infty$ limit.

In table 1 we show data for periodic boundary conditions. These were obtained from diagonalizing H through the standard Arnoldi algorithm [3]. Translation and parity invariance were used to blockdiagonalize H, and lead to matrices of size $\approx 2^L/(2L)$ for L sites. In table 2 data for free boundary conditions are shown. They were obtained by applying the DMRG method [40–42] to the pair contact process [39].

Clearly, the data for both $A_L^{(\mathrm{P})}$ and $A_L^{(\mathrm{F})}$ at finite values of L are, in general, quite far away from unity. We also see that the raw data tend to be closer to unity for smaller values of d. However, since the systematic variation of these amplitudes with L is huge, a precise $L \to \infty$ extrapolation must be performed. We have used the BST extrapolation algorithm [59] which has established itself as a reliable and precise method for the extrapolation of finite-lattice sequences arising in both equilibrium and non-equilibrium critical phenomena. The parameter ω describes the (effective) leading finite-size correction of a sequence $A_L = A_\infty + \mathcal{A}_1 L^{-\omega} + \cdots$ and must be chosen to optimize convergence [3, 59].

In all cases, we find that the extrapolated amplitudes

$$A_\infty^{(\mathrm{P})} := \lim_{L\to\infty} A_L^{(\mathrm{P})} \simeq 1 \qquad A_\infty^{(\mathrm{F})} := \lim_{L\to\infty} A_L^{(\mathrm{F})} \simeq 1 \tag{49}$$

within the numerical accuracy of the extrapolation and in full agreement with equation (46). The need for $L \to \infty$ extrapolation also means that the universal infinite-size amplitudes may be hard to see in, say, Monte Carlo simulations. We also give the effective value of ω for each sequence. In view of the exact result $\omega = 1$ for $p = 1$, see (57), (62), it is satisfying that ω stays close to one.

In general, for a given d convergence is best for p close to one and decreases when p is lowered. The lowest values of p given in table 1 are more or less the smallest ones for which a reliable convergence of the amplitudes could still be observed. In varying d, we see that data converge best for relatively small d and that close to $d = 1$ the crossover towards mean-field behaviour [39] affects the finite-size scaling of the amplitudes. Comparing the data for periodic and free boundary conditions for the same values of p and d, we observe that the $A_\infty^{(\mathrm{F})}$ are closer to unity than the $A_\infty^{(\mathrm{P})}$ for the same value of L (and in contrast to the usual expectation that finite-size corrections should be smallest for periodic boundary conditions). For $p = 1$, these remarks are confirmed analytically, see equations (57), (62).

All in all, the extrapolated amplitudes converge over a large range of values of p and d towards unity, in agreement with (46). Therefore, the PCPD in the inactive phase confirms the universality of the correlation length finite-size scaling amplitude as derived in section 2. Since the entire inactive phase is expected to be in the same universality class, that result should apply even to those portions of the inactive phase where our relatively short chains did not permit us to carry out a precise extrapolation.

(2) Second, we briefly discuss the annihilation–coagulation model (42). It is well known [53, 60–63] that the quantum Hamiltonian $H = H(\alpha, \gamma)$ is similar to the quantum Hamiltonian $H(\alpha + \gamma, 0)$ of pure annihilation. Therefore, equations (45), (46) also apply to this model, independently of α and γ. If we take $\alpha + \gamma = 1$, the steady-state particle density amplitude $\lim_{L\to\infty} L\rho(L) = (1 + \alpha/\gamma)/(1 + 2\alpha/\gamma)$ depends on the branching ratio α/γ and is not universal.

Equations (45), (46) state that for the finite-size amplitude of Γ is independent of the ratio $r = \alpha + \gamma$ of the reaction rate and the diffusion rate d. In the light of the universality

Table 1. Estimates for the normalized amplitude $A_L^{(\mathrm{P})} = L^2\Gamma_L/(2\pi^2 d)$ for several values of p and d and periodic boundary conditions. The rows labelled ∞ give the $L \to \infty$ extrapolations obtained from the BST extrapolation algorithm [59] and ω is the effective correction exponent used in these extrapolations. In some cases the sequences are not monotonic: this is indicated by a * at the value of ω used.

$d = 0.10$	L	$p = 0.16$	$p = 0.25$	$p = 0.50$	$p = 0.75$
	6	0.727 447 5706	1.101 416 0997	1.554 336 3873	1.716 614 4988
	8	0.679 199 2625	0.995 170 4118	1.357 553 7598	1.481 977 4944
	10	0.655 985 9469	0.950 543 1819	1.264 899 2305	1.363 137 2237
	12	0.648 003 5923	0.931 854 2215	1.211 075 9662	1.291 306 9885
	14	0.648 326 5043	0.924 701 9281	1.175 771 0267	1.243 193 8517
	16	0.653 099 0879	0.922 980 0785	1.150 754 7386	1.208 715 7132
	18	0.660 255 1037	0.923 896 6184	1.132 063 0670	1.182 796 3304
	20	0.668 654 5657	0.926 088 6593	1.117 546 6079	1.162 601 1550
	∞	1.04(3)	1.00(3)	0.999 9(1)	1.000 1(2)
	ω	1*	1.11*	1	1.0032
$d = 0.30$	L	$p = 0.20$	$p = 0.30$	$p = 0.50$	$p = 0.75$
	6	0.339 373 6439	0.556 511 9224	0.844 899 9662	1.020 574 3378
	8	0.370 839 6385	0.601 675 4416	0.866 477 2095	1.016 477 5547
	10	0.400 127 4702	0.638 527 9575	0.883 674 5934	1.013 732 8840
	12	0.428 782 3558	0.669 897 9484	0.897 565 6827	1.011 822 6252
	14	0.456 239 1902	0.696 709 7472	0.908 838 0138	1.010 411 7821
	16	0.482 057 3931	0.719 771 9798	0.918 074 4129	1.009 319 8954
	18	0.506 069 2639	0.739 768 2858	0.925 731 1017	1.008 445 2275
	20	0.528 275 7026	0.757 245 0703	0.932 153 8891	1.007 726 2607
	∞	0.96(4)	1.000 1(1)	1.000 0(3)	0.999 99(3)
	ω	1.085	1.074	1	1
$d = 0.50$	L	$p = 0.30$	$p = 0.40$	$p = 0.50$	$p = 0.99$
	6	0.263 446 3944	0.359 404 3077	0.436 287 1259	0.595 044 1871
	8	0.307 102 2508	0.415 675 3699	0.497 526 3719	0.658 240 3419
	10	0.348 030 0086	0.464 943 2503	0.548 566 8186	0.705 423 5500
	12	0.386 135 3468	0.507 628 2318	0.590 971 5317	0.741 660 3392
	14	0.421 076 3888	0.544 527 4246	0.626 486 5185	0.770 225 8735
	16	0.452 860 1529	0.576 561 6531	0.656 561 5085	0.793 256 8153
	18	0.481 689 0281	0.604 555 9890	0.682 310 5808	0.812 184 8167
	20	0.507 840 8510	0.629 193 3618	0.704 579 0759	0.827 997 0372
	∞	1.00(2)	1.007(2)	0.996(2)	1.000 2(2)
	ω	0.98	1	1.067	0.994
$d = 0.90$	L	$p = 0.50$	$p = 0.75$	$p = 0.90$	$p = 0.95$
	6	0.054 172 2289	0.072 900 0818	0.078 239 0633	0.079 010 3464
	8	0.067 136 3692	0.090 780 2309	0.097 580 9620	0.098 588 1954
	10	0.080 195 4402	0.108 417 0765	0.116 509 3810	0.117 719 1004
	12	0.093 163 6953	0.125 631 1545	0.134 889 3588	0.136 279 1328
	14	0.105 963 5357	0.142 369 2854	0.152 687 4700	0.154 239 3436
	16	0.118 558 9168	0.158 617 7799	0.169 902 7666	0.171 601 4095
	18	0.130 931 1714	0.174 378 5534	0.186 546 8998	0.188 378 8379
	20	0.143 070 2131	0.189 660 5667	0.202 636 8456	0.204 590 0568
	∞	1.01(1)	0.999(2)	1.001(3)	1.001(2)
	ω	1.081	1.08	1.078	1.079

Table 2. Estimates for the normalized amplitude $A_L^{(\mathrm{F})} = L^2\Gamma_L/(\pi^2 d)$ for several values of p and d and free boundary conditions, and the $L \to \infty$ extrapolation. When the DMRG algorithm did not yield stable results the corresponding finite-size entries are left empty.

$p = 0.40$	L	$d = 0.333$	$d = 0.50$	$d = 0.666$	
	12	0.857 257 7379	0.672 574 7038	0.458 393 5580	
	14	0.873 759 0556	0.705 384 0790	0.498 181 5051	
	16	0.886 994 5040	0.732 284 0138	0.532 754 1136	
	18	0.897 825 1485	0.754 778 5176	0.563 035 3770	
	20	0.906 836 1253	0.773 829 2422	0.589 752 4204	
	22	0.914 440 1079	0.790 179 8864	0.613 482 6888	
	24	0.920 935 8777	0.804 358 3176	0.634 689 0106	
	26	0.926 544 7049	0.816 768 0285	0.653 745 5074	
	28	0.931 433 5748	0.827 717 7891	0.670 957 4987	
	30	0.935 731 8117	0.837 449 1423	0.686 576 1177	
	32	0.939 573 3083	0.846 152 2447	0.700 807 8882	
	34	0.942 938 8328	0.853 990 6968	0.713 831 4424	
	∞	0.999(3)	0.999 9(5)	0.999 5(9)	
	ω	1.08	1.024 5	1.029	
$p = 0.50$	L	$d = 0.333$	$d = 0.50$	$d = 0.666$	
	12	0.912 735 0184	0.739 584 3960	0.525 415 1900	
	14	0.923 969 8644	0.768 683 0752	0.565 606 3523	
	16	0.932 734 9799	0.791 983 2846	0.599 694 9840	
	18	0.939 754 7158	0.811 062 5710	0.628 949 6021	
	20	0.945 494 6130	0.826 970 0162	0.654 314 7959	
	22	0.950 270 1952	0.840 432 5820	0.676 506 7894	
	24	0.954 302 0404	0.851 970 8198	0.696 078 0276	
	26	0.957 754 2440	0.861 967 6543	0.713 461 0277	
	28	0.960 729 0383	0.870 709 7768	0.728 999 0177	
	30	0.963 322 6275	0.878 420 2612	0.742 967 9437	
	32		0.885 271 7697	0.755 590 6209	
	34		0.891 392 4472	0.767 051 4417	
	∞	0.999 6(6)	0.999 6(5)	0.999 6(5)	
	ω	1.092 5	1.016 5	1.019 1	
$d = 0.90$	L	$p = 0.60$	$p = 0.70$	$p = 0.80$	$p = 0.90$
	12	0.186 316 7451	0.204 252 8770	0.217 223 7514	0.225 570 5980
	14	0.211 945 6015	0.231 756 9546	0.245 960 0505	0.254 987 3770
	16	0.236 219 9311	0.257 633 3440	0.272 873 7999	0.282 470 6979
	18	0.259 223 7747	0.282 003 4649	0.298 117 9611	0.308 186 7029
	20	0.281 037 2384	0.304 979 4681	0.321 824 9399	0.332 284 8660
	22	0.301 736 7417	0.326 664 5014	0.344 118 9613	0.354 898 9577
	24	0.321 393 9696	0.347 148 2795	0.365 111 7354	0.376 153 4335
	26	0.340 075 9780	0.366 533 6490	0.384 904 6790	0.396 155 2283
	28	0.357 845 5055	0.384 883 3645	0.403 589 9034	0.415 004 6251
	30	0.374 829 5723	0.402 277 8186	0.421 250 4431	0.432 791 4966
	32	0.390 877 4672	0.418 786 3074	0.437 863 9789	0.449 586 3889
	34	0.406 244 1268	0.434 465 0723		
	∞	0.986(20)	0.98(3)	0.983(15)	0.984(15)
	ω	1.09	1.103	1.100	1.099

hypothesis of sections 2 and 3, the observed r-independence of the amplitude $L^2\Gamma$ means that the critical exponents of the pair annihilation process $2A \to \emptyset$ (or the equivalent coagulation process $2A \to A$ [53, 60]) should also be independent of r, i.e. the mean particle density $\rho(t) \sim t^{-\delta}$ with $\delta = 1/2$. While that had been anticipated long ago by many people, exact lattice calculations only exist for $r = 1$, see [30, 47]. The only published verifications of the r-independence of δ we are aware of either used purely numerical methods [62, 64, 65], a real-space renormalization group scheme [66] or other *ad hoc* approximations [67].

The steady-state particle density should scale as

$$\rho_L = D_0 C_2 L^{-\beta/\nu_\perp} Y'\left(0, C_2 h L^{d+\theta-\beta/\nu_\perp}\right)\Big|_{h=0} \tag{50}$$

(borrowing notation from section 2, where the prime indicates the derivative with respect to the second argument and h parametrizes a source of particles). That is standard finite-size scaling without any readily identifiable universal amplitude and is therefore weaker than the forms of sections 2 and 3. It is known from field theory that C_2 is independent of r [54] while it does depend on the branching ratio α/γ [63], which is compatible with our results.

(3) Having checked the scaling function universality in some examples with known behaviour, we now illustrate how this universality might be used as a diagnostic tool. Appealing to the experience gathered in equilibrium systems [4], universal amplitudes might be expected to vary considerably more between distinct universality classes than critical exponents. Therefore, even an approximate determination of universal amplitudes may allow us to conclude on the universality class of the model at hand. Reconsider the phase diagram of the pair contact process in figure 1. Presently, there is no consensus on how many universality classes should be realized along the transition line between the active and inactive phases for $d \neq 0, 1$. As a starting point, we might consider pair mean-field theory, which predicts two distinct universality classes along the two segments of the pair mean-field transition curve [39]. The calculation of both steady-state and time-dependent critical exponents in 1D from simulations [46] appear to be in agreement with this prediction. On the other hand, DMRG studies [39] and different simulations in 1D [44, 45, 68] only find evidence for a single universality class along the transition line.

Here, we consider the ratio $R = E_3/E_2$ of the two lowest non-vanishing eigenvalues of H for free boundary conditions as obtained from the DMRG. We use the Monte Carlo estimates for $p_c(d)$ obtained by Grassberger [45]. R is equal to the ratio of two distinct relaxation times and from equation (24) we expect R to be constant within a given universality class. Our numerical results are shown in figure 2.

At first sight, it might be possible to separate the values of R into two classes, one for smaller values of d (up to $d \approx 0.4$–0.5) and a limit $R_\infty \sim 2$, and one for larger values of d (above $d \approx 0.8$) with a limit $R_\infty \sim 3$–4. The fact that R_∞ is quite independent of d for $0.2 \leqslant d \leqslant 0.4$ confirms the expected universality ($R_\infty = 1$ in the inactive phase because there all levels are twofold degenerate, see appendix).

However, closer inspection reveals that already for $d = 0.5$, the data for R_L for L small start out close to 4 and then begin to cross over to values close to 2. That signals the presence of strong transient effects in this model. In addition, for the values of L for which data exist, the values of R for both $d = 0.8$ and 0.9 are close together and quite close to 4. However, these data, in particular for $d = 0.8$, also show indications that they might also cross over to smaller values of R if L could be increased further. The lattice sizes available are not large enough to be able to distinguish clearly between the possibilities of a single [39, 44, 45, 68] or two [46] transitions, although the possibility of a single transition appears more likely. If there is a change of the universality class along the critical line at all, figure 2 suggests that it certainly should occur for $d > 0.5$.

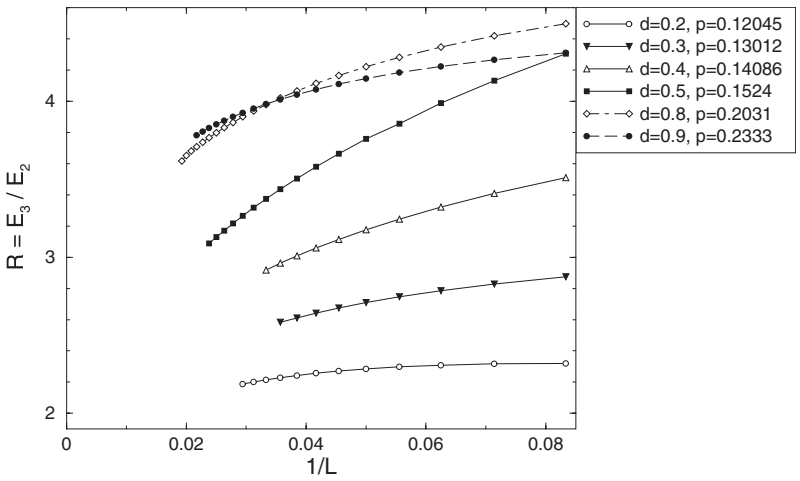

Figure 2. Ratio $R = E_3/E_2$ of the two lowest eigenvalues of H at the critical line $p = p_c(d)$ of the pair contact process, for free boundary conditions and several values of d.

5. Conclusions

In this paper, we have tried to generalize Privman–Fisher [5] universality to (steady-state) phase transitions with dynamical scaling. For equilibrium systems the standard arguments carry over, the main ingredients being translation invariance and hyperscaling. With respect to more standard renormalization group arguments, only the absence of non-universal metric factors in front of the scaling function for $\xi_{\perp,i}$ in equation (23) is new. Equivalently, this may be stated, see equation (24), as the universality of *all* ratios $\xi_{\parallel,i}/\xi_{\parallel,j}$.

Out of equilibrium, new arguments must be sought. In the special case of directed percolation, the peculiar properties equations (33), (35) were seen to be sufficient for amplitude universality. These properties may or may not be available in other universality classes, but we found some numerical evidence in several reaction–diffusion systems that the universal finite-size scaling forms (23), (24) might indeed hold in general. In the annihilation–coagulation model and the pair contact process (inactive phase), we found that the finite-size scaling amplitude of the leading relaxation time is indeed independent of the irrelevant parameters we considered. Further evidence in favour of universality was found by studying the active–inactive transition line in the pair contact process. In addition, our data for the ratio of the two leading relaxation times appear to favour a single universality class along that transition line for $0 < d < 1$. It remains an open question how to derive the universal scaling forms (23), (24) in general non-equilibrium systems.

Recently, the reaction–diffusion process $2A \to A$ and $A\emptyset A \to 3A$ has been studied [69]. If the coagulation rate is equal to the diffusion rate, the model is exactly solvable. It remains in the universality class of diffusion–annihilation for all values of the particle production rate λ. For periodic boundary conditions, the exact amplitude of the leading inverse relaxation time is $\lim_{L\to\infty} L^2\Gamma_L = 2\pi^2 d$, independently of λ, as to be expected from (45), (46).

Finally, upon identification the universal finite-size scaling amplitude of the transverse 'spatial' correlation lengths $\xi_{\perp,i}$, it might be tempting to ask if, in analogy to equilibrium [6–10], there could be relations of universal finite-size scaling amplitudes with some exponents. To answer this question would require a set of worked-out examples on which some hypothesis of this kind could be tried out.

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Appendix: Bethe ansatz calculation

We calculate the lowest gap $\Gamma = E_2$ for $p = 1$ in the pair contact process and derive the amplitude a in (46).

In the $p = 1$ case, only the pair annihilation $AA \to \emptyset\emptyset$ survives. It is well known [52] that in this case, the quantum Hamiltonian can be decomposed $H = H_0 + H_1$ in such a way that the eigenvalue spectrum of H is independent of H_1, namely spec $(H) =$ spec (H_0). The latter is related to the spectrum of the XXZ Heisenberg chain which can be found from the coordinate Bethe ansatz [56, 57].

We begin with the *periodic* case. The spectrum-generating part of H is

$$H_0 = d H_{XXZ}(\Delta, t) + \tfrac{1}{4}(1+d)L \tag{51}$$

where

$$H_{XXZ}(\Delta, t) = -\tfrac{1}{2}\sum_{i=1}^{L}\left[\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \Delta\sigma_i^z\sigma_{i+1}^z + t\sigma_i^z\right] \tag{52}$$

and

$$\Delta = \frac{3d-1}{2d} \qquad t = \frac{1-d}{d}. \tag{53}$$

Since the total spin $S^z := \sum_{i=1}^{L}\sigma_i^z$, commutes with H_{XXZ}, the eigenstates $H_0|\psi_n\rangle = E_n|\psi_n\rangle$ can be classified in terms of the number n of reversed spins, namely $S^z|\psi_n\rangle = (L-2n)|\psi_n\rangle$. The lowest states with $n = 0, 1$ have zero energy and correspond to the two steady states of the model. The lowest gap Γ is found in the sector $n = 2$. From [57], one has

$$E_2 = 2d(2 - \cos k - \cos k') \qquad Lk = 2\pi I - \Theta(k, k') \qquad Lk' = 2\pi I' - \Theta(k', k) \tag{54}$$

where

$$\Theta(k, k') = 2\arctan\frac{\Delta\sin((k-k')/2)}{\cos((k+k')/2) - \Delta\cos((k-k')/2)} \tag{55}$$

and $I, I' = \pm\frac{1}{2}, \pm\frac{3}{2}, \ldots$ are distinct half-integers. The total momentum of the corresponding state is $P = k + k' = 2\pi(I + I')/L'$. The lowest energy gap will have $P = 0$, or $k' = -k$. Furthermore, the lowest energy state corresponds to the choice $I = -I' = 1/2$, as can be checked by considering the special case $\Delta = 0$ (because of the symmetry between k and k', all levels are twofold degenerate). We find

$$\Gamma = 4d(1 - \cos k) \qquad \tan\frac{Lk - \pi}{2} = -\frac{\Delta\sin k}{1 - \Delta\cos k}. \tag{56}$$

For L large, the solution of the second equation (56) is

$$k \simeq \frac{\pi}{L}\left(1 - \frac{2\Delta}{1-\Delta}\frac{1}{L} + \cdots\right). \tag{57}$$

Inserting this into (56), we arrive indeed at the first case of equations (45), (46).

Second, we consider *free* boundary conditions. The spectrum-generating part of H is

$$H_0 = dH_{XXZ}(\Delta, t, r) + \tfrac{1}{4}(1+d)(L-1) \tag{58}$$

$$H_{XXZ}(\Delta, t, r) = -\tfrac{1}{2}\left\{\sum_{i=1}^{L-1}\left[\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \Delta\sigma_i^z\sigma_{i+1}^z\right] + r\left(\sigma_1^z + \sigma_L^z\right) + t\sum_{i=1}^{L}\sigma_i^z\right\} \tag{59}$$

where we used (53) and $r = -t/2$. Again, Γ will be the lowest energy in the $n = 2$ sector. From the Bethe ansatz [56], one has

$$E_2 = 2d(2 - \cos k - \cos k') \qquad \mathrm{e}^{2\mathrm{i}(L-1)k} = \left(\frac{f_{-k}(r,\Delta)}{f_k(r,\Delta)}\right)^2 \mathrm{e}^{-\mathrm{i}\Theta(k,k')+\mathrm{i}\Theta(-k,k')} \tag{60}$$

where $f_k(a,b) = a - b + \mathrm{e}^{\mathrm{i}k}$. A similar equation holds for k', where k and k' are exchanged with respect to (60). The lowest excitations in the $n = 2$ sector are found for $k' = 0$ (up to a twofold degeneracy). Since $r - \Delta = -1$, using (55) and taking the logarithm, we find

$$\Gamma = 2d(1 - \cos k) \qquad Lk = \pi(I+1) - 2\arctan\left(\frac{\Delta}{1-\Delta}\tan\frac{k}{2}\right) \tag{61}$$

where $I = 0, 1, 2, 3, \ldots$. The lowest gap is obtained for $I = 0$, as can be checked for $\Delta = 0$. In analogy to the periodic case, we rewrite the second equation in (61) in the form $\tan((Lk - \pi)/2) = -\Delta/(1-\Delta)\tan(k/2)$. For L large, the solution is

$$k \simeq \frac{\pi}{L}\left(1 - \frac{\Delta}{1-\Delta}\frac{1}{L} + \cdots\right) \tag{62}$$

from which the second case in equations (45), (46) follows.

Evidently, for $\Delta = 0$, that is $d = 1/3$, we recover for both boundary conditions the well known results found from free-fermion methods. A second closed solution exists for $d = 1/2$ and *free* boundary conditions. Then $\Delta = 1/2$ and the second of equations (61) reduces to $(L+1)k = \pi(I+1)$. The lowest gap is obtained for $I = 0$ and we arrive at (47). We also remark that for the $\Delta = 1/2$ XXZ chain with boundary terms such that $U_q(sl(2))$ invariance holds, the Bethe ansatz equation can be solved analytically [58].

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