Comment on "Critical behavior of a two-species reaction-diffusion problem"

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In a recent paper, de Freitas *et al.* [Phys. Rev. E **61**, 6330 (2000)] presented simulational results for the critical exponents of the two-species reaction-diffusion system $A+B\to 2B$ and $B\to A$ in dimension $d=1$. In particular, the correlation length exponent was found as $\nu=2.21(5)$ in contradiction to the well-known relation $\nu=2/d$. In this Comment, the symmetry arguments leading to exact critical exponents for the universality class to which this reaction-diffusion system belongs are concisely reconsidered.

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In a recent paper, de Freitas *et al.* [1] presented a Monte Carlo study of the two-species reaction-diffusion system $A+B\to 2B$ and $B\to A$ [the van Wijland, Oerding, Hilhorst (WOH) model [2]] in dimension $d=1$. They reported the values $\beta=0.435(10)$ and $\nu=2.21(5)$ for critical exponents of the order parameter and the correlation length, respectively. The measurement of the short-time scaling exponent θ' [3] seems consistent with the scaling laws $\theta'=-\eta/z$ and $2\beta/\nu=d+\eta$, using the exact value $z=2$ of the dynamical exponent. The term "exact" means here at least correct as long as the (super) renormalizable model (1) presented below has a nontrivial infrared stable fixed point. Note that an ε expansion is in general not involved. The critical WOH model belongs in general to the universality class of directed percolation (DP) processes coupled to a secondary conserved density called DP-C [4], in analogy to the Model C. In the same manner as the universal behavior of the critical dynamics of a relaxing nonconserved order parameter near equilibrium (Model A) is changed to Model C by the coupling to a conserved density, DP processes are changed to DP-C processes. de Freitas *et al.* assume equal diffusion constants for both species. Therefore, a special DP-C process without cross-diffusion called KSS, and identified by Kree *et al.* [5] several years ago, describes the special system studied here. In the Appendix of their paper, Kree *et al.* show by means of a Ward identity that the correlation length exponent obeys the exact relation $\nu=2/d$. This yields $\nu=2$ in one dimension. Note that the original KSS model consists of the two-species reaction-diffusion system $B\to 2B$, $2B\to B$, $B+C\to C$ with unequal diffusion constants for both species and is therefore microscopically different from the WOH model. However, the authors of [2] show that their model with equal diffusion coefficients renormalizes by coarse graining to the KSS model. Thus, de Freitas *et al.* correctly assume that their simulated WOH model belongs to the KSS universality class. Therefore, the value of ν reported by de Freitas *et al.* turns out to be erroneous as long as one assumes that the symmetry properties of the fixed point are not destroyed in one spatial dimension. Likewise, their conjectured simple fractions for the critical exponents have to be rejected.

Because the arguments leading to exact critical exponents of the DP-C processes are more or less implicit in several papers [2,5], I will reconsider their derivation in this Comment, and show that they all have their roots in particular symmetry properties.

The Langevin dynamics of the DP-C class can be described by the dynamic functional [6,7]

$$\mathcal{J}=\int dt\, d^dx\left\{\tilde{s}\left[\partial_t+\lambda(\tau-\nabla^2+fc)+\frac{\lambda}{2}(gs-\tilde{g}\tilde{s})\right]s+\tilde{c}[\partial_t c-\gamma\nabla^2(c+\sigma s)]-\gamma(\nabla\tilde{c})^2\right\}. \quad (1)$$

Here s and c are the densities of the percolating agent and the conserved field, respectively. In the case of the reaction-diffusion system above, $s\propto n_B$ and $c\propto n_A+n_B$, where n_A and n_B denote the densities of the A and B particles, respectively. The conjugated response fields are denoted by $\tilde{s}$ and $\tilde{c}$. Stability requires $g>2\sigma f$. Green functions (correlation and response functions) are obtained by integrating the fields against a weight factor $\exp(-\mathcal{J})$.

The functional $\mathcal{J}$, Eq. (1), possesses the following symmetries under three transformations involving a constant continuous parameter α:

$$\text{I:}\quad \tilde{c}\to\tilde{c}+\alpha; \quad (2)$$

$$\text{II:}\quad c\to c+\alpha,\quad \tau\to\tau+f\alpha; \quad (3)$$

$$\text{III:}\quad s\to\alpha s,\quad \tilde{s}\to\alpha^{-1}\tilde{s},\quad \sigma\to\alpha^{-1}\sigma,\quad g\to\alpha^{-1}g,\quad \tilde{g}\to\alpha\tilde{g}. \quad (4)$$

Moreover, $\mathcal{J}$ is invariant under the inversion:

$$\text{IV:}\quad \tilde{c}\to-\tilde{c},\quad c\to-c,\quad \sigma\to-\sigma,\quad f\to-f. \quad (5)$$

In the particular case $\sigma=0$, the time reflection

$$\text{V:}\quad \sqrt{g/\tilde{g}}\,s(\mathbf{x},t)\leftrightarrow-\sqrt{\tilde{g}/g}\,\tilde{s}(\mathbf{x},-t),$$
$$c(\mathbf{x},t)\to c(\mathbf{x},-t),\quad \tilde{c}(\mathbf{x},t)\to c(\mathbf{x},-t)-\tilde{c}(\mathbf{x},-t) \quad (6)$$

yields a further discrete symmetry transformation. The symmetry V distinguishes the KSS from general DP-C processes.

Symmetry I results from the conservation property of the field c. Symmetries III and IV show that dimensionless invariant coupling constants and parameters are defined by $u=\tilde{g}g\mu^{-\varepsilon}$, $v=f^2\mu^{-\varepsilon}$, $w=\sigma\tilde{g}f\mu^{-\varepsilon}$, and the ratio of the kinetic coefficients $\rho=\gamma/\lambda$. Here μ^{-1} is a convenient mesoscopic length scale and $\varepsilon=4-d$.

Dimensional analysis and the scaling symmetry III applied to the Green functions $G_{N,\tilde{N};M,\tilde{M}}=\langle[s]^N[\tilde{s}]^{\tilde{N}}[c]^M[\tilde{c}]^{\tilde{M}}\rangle$ gives

$$G_{N,\tilde{N};M,\tilde{M}}=\alpha^{\tilde{N}-N}G_{N,\tilde{N};M,\tilde{M}}\times(\{\mathbf{x},t\},\tau,\alpha^{-1}\sigma,\alpha\tilde{g},\alpha^{-1}g,f,\lambda,\gamma,\mu) \quad (7)$$

$$=\sigma^{\tilde{N}-N}F_{N,\tilde{N};M,\tilde{M}}(\{\mu\mathbf{x},\gamma\mu^2 t\},\mu^{-2}\tau,u,v,w,\rho) \quad (8)$$

$$=(g/\tilde{g})^{(\tilde{N}-N)/2}F'_{N,\tilde{N};M,\tilde{M}}\times(\{\mu\mathbf{x},\gamma\mu^2 t\},\mu^{-2}\tau,u,v,w,\rho), \quad (9)$$

where it is assumed that $\sigma\geqslant 0$ for convenience. Of course, Eq. (8) cannot be used if $\sigma=0$.

The critical scaling properties of the Green functions can be extracted from the invariant functions F and F' by applying the renormalization group. To extract UV-finite quantities from the field theory, one introduces bare fields and parameters and renormalizes by appropriate Z factors. For example, one uses the scheme $s\rightarrow\mathring{s}=Z_s^{1/2}s$, $\tilde{s}\rightarrow\mathring{\tilde{s}}=Z_{\tilde{s}}^{1/2}\tilde{s}$, $\tau\rightarrow\mathring{\tau}=Z_\tau\tau+\mathring{\tau}_c$, $f\rightarrow\mathring{f}=Z_f v^{1/2}\mu^{\varepsilon/2}$, etc. Here $\mathring{\tau}_c$ denotes the critical value of $\mathring{\tau}$. The Z factors have to absorb all the UV infinities (the ε poles in dimensional regularization). They can only depend on the invariant parameters u, v, w, and ρ.

The objects of the calculation are the vertex functions $\Gamma_{\tilde{N},N;\tilde{M},M}$, i.e., the one-particle irreducible amputated diagrams with $\tilde{N}$ $\tilde{s}$-legs, N s-legs, $\tilde{M}$ $\tilde{c}$-legs, and M c-legs. It is easily seen that diagrams with loops do not contribute to vertex functions with $\tilde{M}\geqslant 1$. Thus, these vertex functions are trivial and given by the corresponding terms displayed in the dynamic functional $\mathcal{J}$, Eq. (1). Hence, the renormalizations are trivial:

$$\mathring{\tilde{c}}=\tilde{c},\quad \mathring{c}=c,\quad \mathring{\gamma}=\gamma,\quad \mathring{\sigma}\mathring{s}=\sigma s. \quad (10)$$

Symmetry II in connection with the trivial renormalization of c, Eq. (10), shows that f is renormalized with the same Z factor as τ: $Z_f=Z_\tau$. It follows the simple relation

$$\frac{\tau}{\mu^{\varepsilon/2}}=\frac{(\mathring{\tau}-\mathring{\tau}_c)}{\mathring{f}}v^{1/2}. \quad (11)$$

At a fixed point v_* different from 0 and ∞, τ changes according to this relation by a change of the momentum scale $\mu\rightarrow\mu l$ (holding bare parameters fixed) as $\tau\rightarrow\tau(l)=\tau l^{\varepsilon/2}$. Thus, one finds from the Eqs. (8,9) the scaling properties of the Green functions at a fixed point with finite values for u_*, v_*, w_*, and ρ_* different from 0 and ∞ (the existence of such fixed points can be demonstrated in the ε expansion [2,4,5])

$$G(\{\mathbf{x},t\},\tau)=l^{\delta_G}G(\{\mu l\mathbf{x},\gamma\mu^2 l^2 t\},\mu^{-2}\tau/l^{2-\varepsilon/2}). \quad (12)$$

In Eq. (12) $\delta_G=(N+\tilde{N}+M+\tilde{M})d/2+(N\eta+\tilde{N}\tilde{\eta})/2$ denotes the scaling exponent of G. δ_G combines the normal and anomalous dimensions of the fields involved in the Green function G. From Eq. (12) one can gather the exact values of the dynamical exponent $z=2$ and the correlation length exponent $\nu=1/(2-\varepsilon/2)=2/d$.

The renormalization of quantities invariant under the transformation defining symmetry III, like F or F', involve only the product of the field renormalizations $Z=Z_{\tilde{s}}Z_s$. Thus, one has a freedom to define one of these factors. With respect to Eqs. (8) and (10), it is convenient to choose the trivial renormalization $\mathring{\sigma}=\sigma$ together with $Z_s=1$. Then the Green functions G have the same scaling properties under renormalization as the invariant functions F. One could also define $Z_s\neq 1$ and renormalize $\mathring{\sigma}=Z_s^{-1/2}\sigma$. The renormalization properties of F are not affected by this choice. Hence, one finds the same critical scaling properties of the correlation and response functions as for the previous one. It follows the anomalous dimension of the field s as $\eta=0$. Then the anomalous dimension $\tilde{\eta}$ of the response field $\tilde{s}$ is given by the logarithmic derivative of Z with respect to the momentum scale μ at the fixed point. $\tilde{\eta}$ is the only scaling exponent that one has to determine by perturbation theory.

For the KSS processes σ vanishes and one cannot follow the strategy of the last paragraph. However, for the KSS processes the time reflection symmetry V can be explored. With respect to this symmetry and Eq. (9), it is now convenient to choose the ratio $\mathring{\tilde{g}}/\mathring{g}=\tilde{g}/g$ trivially renormalized together with $Z_s=Z_{\tilde{s}}=Z^{1/2}$. Then the Green functions G have the same critical scaling as the invariant functions F'. The logarithmic derivative of Z at the fixed point yields in this case the value of $\eta=\tilde{\eta}$.

In summary, the DP-C processes offer exact relations for some critical exponents including $z=2$ and $\nu=2/d$. In the KSS case, one has $\eta=\tilde{\eta}$ as in DP, but with another value. In the more general case with cross-diffusion $\sigma\neq 0$ (and $\sigma f<0$) one finds $\eta=0$, which yields via the relation $\beta=\nu(d+\eta)/2$ the exact order parameter exponent $\beta=1$. The discrepancy with the exact and the simulational result for ν by roughly 10% may have the origin in corrections to scaling. It is therefore desirable that the authors reconsider their simulations and provide a careful analysis of such corrections. Another possible, though unlikely source of the discrepancy, is that in such low dimensions as $d=1$ the membership of the simulated WOH model to the KSS universality class is spoiled. This may arise if further symmetry-breaking operators become relevant. Relevance is defined here with respect to the nontrivial fixed point. The relevance of quartic terms for $d<2$ in the dynamic functional (1) with respect to the Gaussian fixed point is not a criterium for that. Additional relevant quartic terms crucially differentiate between the WOH and the KSS model and would destroy any of the exact scaling properties derived from the dynamic functional $\mathcal{J}$. In particular, also the relations $\eta=\tilde{\eta}$, $z=2$, and $\theta'=-\eta/z$, used by the authors of [1], would become doubtful.

Note added in proof. A recent Monte Carlo simulation [8] shows that indeed $\nu=2$ in one spatial dimension.

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