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

Hans-Karl Janßen

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

(March 21, 2022)

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 $A + B \rightarrow 2B$ and $B \rightarrow A$ 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 $\theta'$ 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 critical reaction-diffusion system above belongs in general to the universality class of directed percolation (DP) processes coupled to a secondary conserved density that I call DP-C in analogy to the Model C. In the same manner as the universal behavior of the critical dynamics of a relaxing non-conserved 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 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 $\nu$ cannot be correct. 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 [3, 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

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

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

I: \hspace{1cm} \tilde{c} \rightarrow \tilde{c} + \alpha ;

II: \hspace{1cm} c \rightarrow c + \alpha , \hspace{0.5cm} \tau \rightarrow \tau + f \alpha ;

III: \hspace{1cm} s \rightarrow \alpha s , \hspace{0.5cm} \tilde{s} \rightarrow \alpha^{-1} \tilde{s} , \hspace{0.5cm} \sigma \rightarrow \alpha^{-1} \sigma , \hspace{0.5cm} g \rightarrow \alpha^{-1} g , \hspace{0.5cm} \bar{g} \rightarrow \alpha \bar{g} .

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

IV: \hspace{1cm} \tilde{c} \rightarrow -\tilde{c} , \hspace{0.5cm} c \rightarrow -c , \hspace{0.5cm} \sigma \rightarrow -\sigma , \hspace{0.5cm} f \rightarrow -f .

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

V: \hspace{1cm} \sqrt{g/g} s(x, t) \leftrightarrow -\sqrt{g/g} \tilde{s}(x, -t) , \\
\hspace{1cm} c(x, t) \rightarrow c(x, -t) , \hspace{0.5cm} \tilde{c}(x, t) \rightarrow c(x, -t) - \tilde{c}(x, -t) .


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 \( u = \tilde{g} \mu \varepsilon^{-1}, v = f^2 \mu \varepsilon^{-3}, w = \sigma \tilde{f} \mu \varepsilon^{-4} \), and the ratio of the kinetic coefficients \( \rho = \gamma / \lambda \). Here \( \mu^{-1} \) is a convenient mesoscopic length scale and \( \varepsilon = 4 - d \).

Dimensional analysis and the scaling symmetry III applied to the Green functions \( G_{N,N;M,M}^\tau = ([s]^N[M]^M[c]^M) \)
gives

\[
G_{N,N;M,M}^\tau = \alpha_{N-N}^N G_{N,N;M,M}^\tau \left( \left\{ \{x(t), \tau, \alpha^{-1} \sigma, \alpha^{-1} g, f, \lambda, \gamma, \mu \right\} \right)
\]

\[
= \sigma_{N-N}^N F_{N,N;M,M}^\tau \left( \left\{ \{\mu x, \gamma \mu^2 t, \mu^{-2} \tau, u, v, w, \rho \right\} \right)
\]

\[
= (g/g)(\tilde{N}-N)/2 F_{N,N;M,M}^\tau \left( \left\{ \{\mu x, \gamma \mu^2 t, \mu^{-2} \tau, u, v, w, \rho \right\} \right)
\]

where it is assumed that \( \sigma \geq 0 \) for convenience. Of course, Eqn. (3) 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 and \( \tilde{\sigma} \) parameters \( \mu \rightarrow \tilde{\sigma} \), \( \gamma \rightarrow \gamma \tilde{\sigma} \), \( \mu \rightarrow \mu \tilde{\sigma} \), \( \rho \rightarrow \rho \tilde{\sigma} \), and \( \sigma \rightarrow \sigma \tilde{\sigma} \). Here \( \tilde{\sigma} \) denotes the critical value of \( \sigma \). The Z-factors have to absorb all the UV-infinities (the \( \varepsilon \)-poles in dimensional regularization). They can only depend on the invariant parameters \( u, v, w, \) and \( \rho \).

The objects of the calculation are the vertex functions \( \Gamma_{N,N;M,M}^\tau, \) i.e., the one-particle irreducible amputated diagrams with \( N \) \( \tilde{s} \)-legs, \( N \) \( s \)-legs, \( M \) \( \tilde{c} \)-legs, and \( M \) c-legs. It is easily seen that diagrams with loops do not contribute to vertex functions with \( M \geq 1 \). Thus, these vertex functions are trivial and given by the corresponding terms displayed in the dynamic functional \( \mathcal{J} \), Eqn. (4). Hence, the renormalizations are trivial:

\[
\tilde{c} = c, \quad \tilde{\gamma} = \gamma, \quad \tilde{\sigma} \tilde{s} = \sigma s
\]

Symmetry II in connection with the trivial renormalization of \( c \), Eqn. (5), shows that \( f \) is renormalized with the same \( Z \)-factor as \( \tau \): \( Z_f = Z_\tau \). It follows the simple relation

\[
\tau / \mu^{3/2} = (\tau - \tau_\eta) / f^{3/2}
\]

At a fixed point \( \tau_\eta \) different from 0 and \( \infty \), \( \tau \) changes according to this relation by a change of the momentum scale \( \mu \rightarrow \mu / \tilde{s} \) (holding bare parameters fixed) as \( \tau \rightarrow \tau / \mu^{3/2} \). Thus, one finds from the Eqs. (8) and (9) the scaling properties of the Green functions at a fixed point with finite values for \( u_\eta, v_\eta, w_\eta, \) and \( \rho_\eta \), different from 0 and \( \infty \) (the existence of such fixed points can be demonstrated in the \( \varepsilon \) expansion).

In Eqn. (12) \( \delta_G = (N + \tilde{N} + M + \tilde{M})/d \) denotes the scaling exponent of \( G \). \( \delta_G \) combines the normal and anomalous dimensions of the fields involved in the Green function \( G \). From Eqn. (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 \( Z = Z_f Z_\tau \). 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 \( \tilde{\sigma} = \sigma \) together with \( Z_\eta = 1 \). 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 \( \tilde{\sigma} = Z_s^{-1/2} \sigma \). 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 \( \mu \) at the fixed point. \( \tilde{\eta} \) is the only scaling exponent that one has to determine by perturbation theory.

For the KSS processes \( \sigma \) vanishes and one cannot follow the strategy of the last paragraph. However, for the KSS processes the time inversion symmetry \( \mathcal{V} \) can be explored. With respect to this symmetry and Eqn. (1) it is now convenient to choose the ratio \( \tilde{\eta} / \tilde{\eta} = \tilde{g} / g \) trivially renormalized together with \( Z_s = Z_\tilde{s} = Z_s^{1/2} \). 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 $\sigma \neq 0$ (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 $\nu$ 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.

[1] J. E. de Freitas, L. S. Lucena, L. R. da Silva, and H. J. Hilhorst, Phys. Rev. E 61, 6330 (2000).
[2] H. K. Janssen, B. Schaub, and B. Schmittmann, Z. Phys. B: Cond. Mat. 73, 539 (1989).
[3] F. van Wijland, K. Oerding, and H. J. Hilhorst, Physica A 61, 6330 (2000).; K. Oerding, F. van Wijland, J. P. Leroy, and H. J. Hilhorst, cond-mat/9910351 (unpublished).
[4] H. K. Janssen, unpublished.
[5] R. Kree, B. Schaub, and B. Schmittmann, Phys. Rev. A 39, 2214 (1989).
[6] H. K. Janssen, Z. Phys. B: Cond. Mat. 23, 377 (1976); in Dynamical Critical Phenomena and Related Topics (Lecture Notes in Physics, Vol. 104), edited by C. P. Enz, (Springer, Heidelberg, 1979).; in From Phase Transitions to Chaos, edited by G. Györgyi, I. Kondor, L. Sasvári, and T. Tél, (World Scientific, Singapore, 1992).
[7] C. De Dominicis, J. Phys. (France) Colloq. 37, C247 (1976).