Erratum: Renormalization Group Study of the $A + B \to \varnothing$ Diffusion-Limited Reaction[1]

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A recent argument of Oerding shows that our calculation of the quantity Δ, which determines the amplitude of the asymptotic decay of the particle density in $2 < d < 4$, was in error. Instead it is simply given by $\Delta = n_0$, the initial density, for uncorrelated initial conditions.

In recent years much progress has been made in applying field-theoretic renormalization-group methods to models of diffusion-limited chemical reactions. One such example was a study by the present authors of the $A + B \to \varnothing$ annihilation reaction with random initial conditions and equal particle densities.[1] Our purpose here is to correct a mistake contained in this worked and to revise the conclusions accordingly. In particular, we now find for spatial dimensions $2 < d < 4$ that the A, B particle densities decay in time with the universal form

$$\langle a(t) \rangle = \langle b(t) \rangle \sim \frac{\sqrt{n_0}}{\pi^{1/2}(8\pi)^{d/4}} (Dt)^{-d/4} \tag{1}$$

where $\langle a(0) \rangle = \langle b(0) \rangle = n_0$, and D is the diffusion constant. This amplitude is exactly that obtained in the approximate calculation of

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Toussaint and Wilczek,[2] and the initial density dependence is the same as found by Bramson and Lebowitz in the limit of an instantaneous reaction.[3] In our previous study we identified nonuniversal corrections to the amplitude in (1) of order $n_0^{d/2}$.[1] However, in analogy with an argument of Oerding[4] for the same reaction in a random shear flow, it can be shown quite generally that the sum of all such corrections in fact vanishes. We now briefly paraphrase his arguments in the context of the present problem.

In general one begins with a master equation description of the diffusive and reactive particle dynamics. This is mapped to a field theory using by now standard techniques.[1, 5, 6] It is convenient to replace the fields $a(x, t)$ and $b(x, t)$ with their sum (ϕ) and difference (ψ), resulting in the action[4]

$$S = \int d^d x \, dt \{ \bar{\phi}(\partial_t - \nabla^2) \, \phi + \bar{\psi}(\partial_t - \nabla^2) \, \psi + \lambda_1 \bar{\phi}(\phi^2 - \psi^2)$$

$$+ \lambda_2 (\bar{\phi}^2 - \bar{\psi}^2)(\phi^2 - \psi^2) - n_\phi \, \delta(t)\bar{\phi} \} \tag{2}$$

The relation between the couplings in (2) and the original master equation parameters is given in Ref. 1. Note that the diffusion constant is absorbed into a resealing of time, and the conjugate fields $\bar{\phi}$ and $\bar{\psi}$ are introduced in the mapping.

The renormalization group (RG) analysis reveals that the critical dimension for the coupling λ_2 is $d_c = 2$, i.e., λ_2 is irrelevant for $d > 2$. Since the dynamic RG relates evolution in time to renormalization group flows, one finds that the asymptotic behavior of the theory is given for $d > 2$ by an effective action of the form

$$S_{\text{eff}} = \int d^d x \, dt \, \{ \bar{\phi}(\partial_t - \nabla^2) \, \phi + \bar{\psi}(\partial_t - \nabla^2) \, \psi + \lambda_{\text{eff}} \bar{\phi}(\phi^2 - \psi^2)$$

$$- \delta(t) \, [n_\phi \bar{\phi} + \tfrac{1}{2} \Delta \bar{\psi}^2 + \cdots] \} \tag{3}$$

Under the renormalization flows for $d > 2$ one has $\lambda_1 \to \lambda_{\text{eff}}$, and, more importantly, new initial terms are generated, such as $\tfrac{1}{2} \Delta \bar{\psi}^2$. While many such terms may appear and be relevant for $d < 4$, it was shown in Ref. 1 that for $2 < d < 4$ the asymptotic behavior of the density and correlation functions is determined solely by Δ. Hence we now focus on the generation of this coupling. [For $d > 4$ one obtains the rate equation result $\langle a(t) \rangle \propto 1/\lambda_{\text{eff}} t$.]

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[4] Note the sign error in the couplings λ_i in Eqs. (2.18) and (2.27) or Ref. 1.

Denote the sum of all diagrams in an expansion of (2) which terminate at time t with two external ψ lines by $\bar{\psi}(t)^2 \, \Pi(t)$. This is illustrated schematically in Fig. 4a of Ref. 1. Since $\Pi(t)$ is damped for times $t \gg 1/n_\phi \lambda_1$, the replacement

$$\bar{\psi}(t)^2 \Pi(t) \simeq \bar{\psi}(0)^2 \, \delta(t) \int_0^\infty dt' \; \Pi(t') \equiv \tfrac{1}{2} \Delta \bar{\psi}(0)^2 \, \delta(t) \tag{4}$$

is valid for calculating asymptotic quantities, and serves to define Δ.

The sum of all such diagrams containing no loops is given below in Fig. 1a and yields a contribution $\Delta^{(a)} = n_0$, the initial density. Here, following the notation of Ref. 1, the dashed line represents the ψ propagator, the heavy solid line is the ϕ classical (tree-level) response function, which is the ϕ propagator dressed by the initial density, and the wavy line is the classical density. Three- and four-point vertices have coupling constants λ_1 and λ_2, respectively, with signs which can be determined from (2). In Ref. 1 we assumed that all other diagrams in $\Pi(t)$, except those which dressed the λ_2 vertex, could be accounted for by taking $\lambda_1 \to \lambda_{\text{eff}}$ in the tree-level diagrams. This left $\Delta^{(a)}$ unchanged, and the corrections were found to yield an expansion in powers of n_0 of the form $\Delta = n_0 - C' n_0^{d/2} + \cdots$, with C' nonuniversal [see Eq. (1.5) in Ref. 1]. However, Oerding has shown that Δ can be calculated exactly from the full action (2), with the result[4]

$$\Delta = n_0 \tag{5}$$

Since Δ itself is not renormalized,[1] this must be the correct value for the effective action (3), in contradiction with the previous result.

Oerding's result follows from observing that all diagrams in $\Pi(t)$ belong to one of the three groups in Fig. 1. The shaded area represents the same set of diagrams in Fig. 1b as in Fig. 1c. These may be attached to the highlighted vertex (represented by a dot) by either two ψ or two ϕ lines:
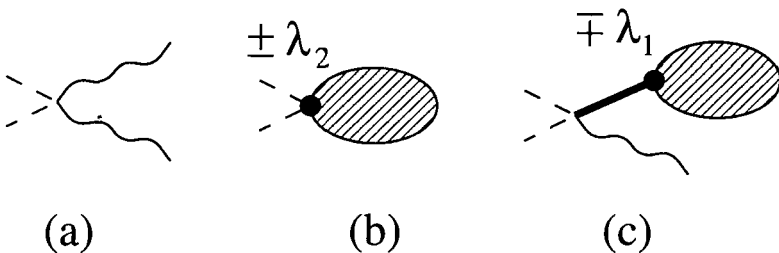

$\pm \lambda_2$ $\mp \lambda_1$

(a)   (b)   (c)

Fig. 1.   Diagrams which contribute to $\Pi(t)$, hence to Δ. The symbols are defined in the next and in Ref. 1.

in either case, the sign of the λ_2 vertex in Fig. 1b is the opposite of the λ_1 vertex in Fig. 1c, as can be confirmed by S in (2). Therefore, writing the contribution from Fig. 1b as

$$\Delta^{(b)} = \lambda_2 \int_0^\infty dt \, f(t) \tag{6}$$

implies that the contribution from Fig. 1c is

$$\Delta^{(c)} = \int_0^\infty dt \, (2\lambda_2) \frac{n_\phi}{1 + n_\phi \lambda_1 t} \int_0^t dt' \left(\frac{1 + n_\phi \lambda_1 t'}{1 + n_\phi \lambda_1 t} \right)^2 (-\lambda_1) f(t')$$

$$= -\lambda_2 \int_0^\infty dt' \, f(t') \tag{7}$$

Hence $\Delta = \Delta^{(a)}$, which leads to (5).

Using the correct and universal result for Δ in the analysis of Ref. 1 yields the asymptotic density (1). In Ref. 1 we also derived the correlation functions and the density in the case of unequal diffusion constants $D_A \neq D_B$. Since these results are expressed in terms of Δ, they may be regarded as correct and universal once the substitution (5) is made. However, we stress that these results are universal only for truly random initial conditions. Correlations initially present are expected to modify Δ in a nonuniversal way.

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