Renormalisation of fluctuation effects in the A+A to A reaction

LETTER TO THE EDITOR

Renormalisation of fluctuation effects in the $A + A \to A$ reaction†

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Abstract. The field theoretical description of the $A + A \to A$ reaction is exactly renormalised to all orders in perturbation theory. It is confirmed that it belongs to the same universality class as the $A + A \to \varnothing$ reaction, and that the concentration decay like $t^{-d/2}$ for space dimensionality d smaller than two and like $(\ln t/t)$ for $d = 2$ are exact results.

The reaction $A + A \to A$ can be considered as the crudest model of irreversible aggregation. It corresponds to considering only the reduction in cluster density as the evolving quantity, if all size dependences of the reaction rate and diffusion constant are neglected. It has been conjectured, on the basis of computer simulation, that it belongs to the same universality class as the $A + A \to \varnothing$ reaction (Kang and Redner 1984). The mean-field rate equations for both reactions are in fact the same and read

$$\frac{dc(t)}{dt} \propto c^2(t) \tag{1}$$

where $c(t)$ is the reactant concentration. This equation implies that $c(t)$ asymptotically decays like t^{-1}. Computer simulations and heuristic considerations have led to the conclusion that this behaviour should be exact, even in the presence of diffusion and spatial density fluctuations, if the space dimensionality d is larger than two; at $d = 2$ one should have

$$c(t) \propto (\ln t/t) \tag{2}$$

whereas for $2 > d \geqslant 1$ one should have

$$c(t) \propto t^{-d/2} \tag{3}$$

(Doi 1976b, Toussaint and Wilszek 1983, Torney and McConnell 1983, Meakin and Stanley 1984, Kang and Redner 1984).

The aim of this letter is to confirm these results by means of an exact renormalisation, to all orders of perturbation theory, of the field theoretical description of this reaction, obtained by means of the path integral representation of birth–death processes introduced by Doi 1976a (for a pedagogical introduction, see, e.g., Peliti 1985).

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† This work is dedicated to Kiho Kang (1957-85).
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We consider the general reaction scheme

$$A + A \xrightarrow{\lambda} A \qquad A + A \xrightarrow{\mu} \varnothing \tag{4}$$

which encompasses both reactions with a suitable choice of the rates λ and μ. Introducing diffusion (with diffusion rate ν) and the annihilation a_r and creation π_r operators on a simple cubic d-dimensional lattice $\{r\}$, the process is presented by the following Liouvillian operator:

$$L = \sum_r \left(\nu \sum_e (\pi_{r+e} - \pi_r) a_r - \lambda (\pi_r - 1) \pi_r a_r^2 - \mu (\pi_r^2 - 1) a_r^2 \right). \tag{5}$$

The vectors e are nearest-neighbour vectors. To this operator corresponds a Lagrangian which in the continuous limit takes the form

$$\mathcal{L} = \int d^d r \left(\hat{\psi} \frac{\partial \psi}{\partial t} - \hat{\psi} \nabla^2 \psi + \tfrac{1}{4} \gamma_0 \hat{\psi}^2 \psi^2 + \tfrac{1}{2} \sigma_0 \hat{\psi} \psi^2 \right) \tag{6}$$

where γ_0 and σ_0 can easily be expressed in terms of λ and μ. The fact that all processes of the type of equation (4) correspond to the same Lagrangian density confirms that they all belong to the same universality class. Dimensional analysis shows that both coupling constants γ_0 and σ_0 have inverse length dimension equal to $(2 - d)$, and hence that d appears as the upper critical dimension. One should worry about the appearance of other relevant interactions not contained in equation (6). Let us remark that both interaction terms in equation (6) do not increase the number of $\hat{\psi}$ (outgoing) fields with respect to that of ψ (incoming) fields. Perturbation theory can therefore only generate couplings of the form $\hat{\psi}^m \psi^n$ with $n \geq m$. Now dimensional analysis shows that all such couplings are irrelevant around $d = 2$ except those already contained in equation (6).

It is remarkable that the Lagrangian (6) can be exactly renormalised to all orders in perturbation theory. All terms in perturbation theory are represented by diagrams, in which the propagator $\langle \hat{\psi}(r', t') \psi(r, t) \rangle$ is represented by a line directed towards (r, t) and the interaction vertices proportional to γ_0 and σ_0 have both two incoming lines and two or one outgoing lines respectively. One may check that no diagrams renormalising the propagator arise. One only has to renormalise the coupling constants, i.e. the reaction rates. It turns out that the only diagrams which renormalise them are the 'parquet' diagrams shown in figure 1, where the last vertex corresponds to γ_0 or σ_0 depending on whether one is renormalising γ or σ. The sum of the diagrams shown in figure 1 is given by

$$J(k, \omega) = [1 + \gamma_0 I(k, \omega)]^{-1} \tag{7}$$

where $I(k, \omega)$ is the contribution of the loop, which is readily computed to be

$$I(k, \omega) = \tfrac{1}{2} K_d \frac{\pi}{\sin(\tfrac{1}{2} \pi d)} (-i\omega + \tfrac{3}{4} k^2)^{(d/2)-1} \tag{8}$$
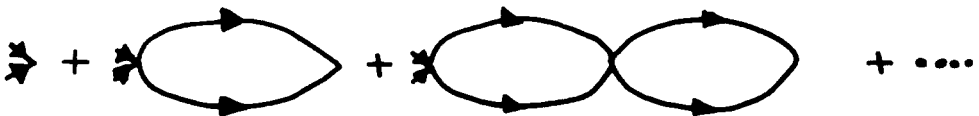

Figure 1. The 'parquet' diagrams which renormalise the reaction kernel.

where $K_d = 2^{1-d}\pi^{-d/2}/\Gamma(d/2)$. Equation (7) implies the following expression for the renormalised reaction rates:

$$(\gamma_r, \sigma_r) = (\gamma, \sigma)J(k, \omega). \tag{9}$$

This corresponds to a singular time- and space-dependent reaction kernel. In the limit of small frequency and wavenumber, for $d < 2$, one has in fact,

$$\gamma_r \sim (k^2)^{1-d/2} f(\omega/k^2). \tag{10}$$

By imposing on all terms in the Lagrangian (6) to scale in the same way, one recovers equation (3). By the same token, going to the limit $d \to 2$ in equation (9) we obtain

$$\gamma_r \sim [\ln(-i\omega + 3k^2/4)]^{-1} \tag{11}$$

which is easily seen to correspond to equation (2). These results are confirmed by a renormalisation group analysis, which can be carried out in the usual way.

We have shown how the field theoretical description of the reaction $A + A \to A$ can be exactly renormalised in order to put the following conjectures on a firm basis:

(i) that it belongs to the same universality class as the $A + A \to \varnothing$ reaction;

(ii) that the upper critical dimension is two, where the concentration $c(t)$ asymptotically behaves like $(\ln t/t)$;

(iii) that below two dimensions, $c(t)$ behaves like $t^{-d/2}$.

This confirms the power of field theoretical methods in reaction kinetics. It is to be hoped that they will find successful application to more complicated reactions.

References

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