Generalized Reaction-Diffusion: a microscopic approach

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In systems where diffusing particles are subject to a reactive process, diffusion and reaction are coupled and reaction-diffusion (R-D) phenomena are described at the macroscopic level by R-D equations. For instance, for an anihilation process such as $A \to 0$, the classical R-D equation reads

$$\frac{\partial}{\partial t} f\,(r;t) = D\,\frac{\partial^2}{\partial r^2} f\,(r;t) \;-\; k\,f\,(r;t)\;, \tag{1}$$

where D denotes the diffusion coefficient and k the reactive rate. The classical equation (1) yields a steady state solution showing exponential decay in space $f\,(r) \;=\; f(0)\,\exp\left(-\sqrt{\frac{k}{D}}\,|r|\right)$.

However in most natural systems where it seems logical to use the language of reaction-diffusion, non-classical distributions are observed where the steady state shows non-exponential behavior e.g. when the particles encounter obstacles in the medium or because the reactive process is hindered or enhanced by concentration effects. So a general description of R-D phenomena requires a generalization for both diffusion and reaction.

We develop a microscopic approach by generalizing Einstein's master equation with a reactive term and we show how the mean field formulation leads to nonlinear R-D equations with non-classical solutions. For the n-th order annihilation reaction $A + A + A + ... + A \to 0$, the generalized reaction-diffusion equation (with no drift) reads

$$\frac{\partial}{\partial t} f\,(r;t) = \frac{\partial}{\partial r}\,D\,\frac{\partial}{\partial r} f^{\alpha}\,(r;t) -\; k\,f^{n}\,(r;t)\;, \tag{2}$$

giving typical solutions $f(r) \;=\; f(0)\,(1 + C_{\alpha,n}\,(D,k)\,r)^{\frac{-2}{n-\alpha}}$ with long range power law behavior showing the relative dominance of sub-diffusion over reaction effects or conversely leading to finite support because diffusion is slow and extinction is fast. Examples of morphogen gradient formation in biological systems are discussed.[1]

[1]J.P. Boon, J.F. Lutsko and C. Lutsko, *Phys. Rev. E*, **77**, 051103 (2012)