Reaction-Diffusion Models in One Dimension

1. Overview of Problems & Techniques

Course overview:

* Problems & techniques
  - ▽ Reaction/Diffusion-controlled limits
  - ▽ Anomalous kinetics: Why $d=1$?
  - ▽ Fluctuations @ all length scales – trapping – $A+B\to\emptyset$.
  - ▽ Fluctuations in number space – Fisher front.
  - △ Effective reaction-order/rate
  - △ Scaling/Dimensional analysis
  - △ Reaction-diffusion equations
* One-species diffusion-limited coalescence, $A+A\to A$, and the Method of Empty Intervals
* $A+A\to\emptyset$ and other advanced applications of "empty intervals"
* Open challenges

Diffusion time: t_D – typical time for "particles" to meet

Reaction time: t_R – typical time for particles to react, when held within reaction range from one another.

Reaction-Controlled: $t_R \gg t_D$

Diffusion-Controlled: $t_D \gg t_R$

→ Rate eqs. / Law of mass action

reaction order

$$nX + mY \rightarrow \text{products} \rightarrow [\dot{X}] = -nk[X]^n[Y]^m$$

rate constant

→ Fluctuation-dominated

$\boxed{\text{no coherent approach}}$

Anomalous kinetics (different from reaction-controlled)

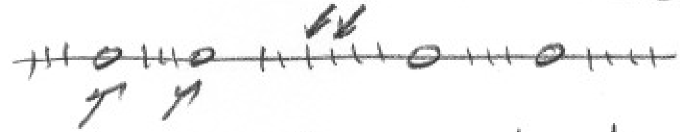
<u>Most</u> anomalous for $d=1$

[upper critical dimension]

Role of fluctuations and examples of anomalous kinetics

random-walkers

(a) trapping



Donsker-Varadhan

$\boxed{\text{Abel prize, 2007; Large deviations}}$

traps at concentration c

Reaction-limited: $S(t) \sim e^{-ct}$

Diffusion-limited:

$$\begin{cases} \text{Prob. of trap-free gap of size } L: ce^{-cL} \\ \text{survival in gap of size } L: e^{-Dt/L^2} \quad \underline{\text{exercise}} \end{cases}$$

$$S(t) = \int_0^\infty e^{-Dt/L^2} ce^{-cL} \, dL \sim e^{-t^{1/3}} \quad (\underline{\text{exercise}})$$

→ anomalous kinetics in all d:

$S(t) \sim e^{-t^{d/d+2}}$ (most anomalous for $d=1$)

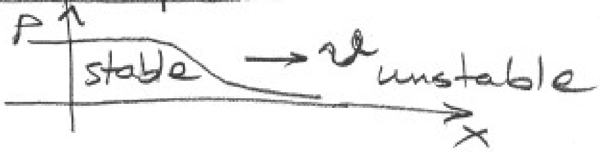
→ result of fluctuations in the size of trap-free regions

(b) $A+B \to \phi$ ($\overset{\text{inert}}{\text{products}}$)

$$\rho \sim t^{-d/4} \qquad d_c = 4 \quad \left(\begin{array}{c} d=1 \\ \text{most} \\ \text{anomalous}\end{array}\right)$$

<u>Fluctuation in number space</u>

(c) Fisher front



ϑ inacurate when one assume ρ continuous (Also, with <u>particles</u> wave front has <u>finite</u> support).

* <u>Exercise</u>: radiactive decay $A \to \phi$
continuum vs. particle kinetics

<u>Techniques</u>

$A + A \to A$ <u>Reaction-limited</u>

$$\dot{\rho} = -k\rho^2 \;\to \text{exercise}$$

$$\boxed{\rho \sim \frac{1}{kt}}, \quad kt \gg \rho_0^{-1}$$

<u>Diffusion-limited</u>

Dimensional analysis:

$$[D] = \frac{L^2}{T}, \quad [t] = T \Rightarrow \underset{[\rho] = \frac{1}{L^d}}{\rho} \sim (Dt)^{-d/2}$$

* But notice assumptions !!

Effective rate eqs.

effective order

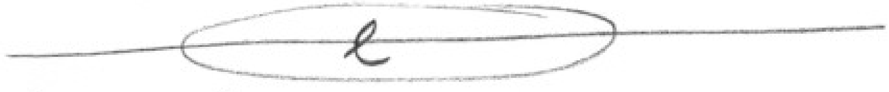
$$\dot{\rho} = -\rho^{3} \rightarrow \rho \sim 1/\sqrt{t} \quad \text{(for } d=1\text{)}$$

or $$\dot{\rho} = -\left(\frac{1}{\sqrt{t}}\right)\rho^{2} \rightarrow \rho \sim 1/\sqrt{t}$$

effective rate

<u>ad-hoc</u>

<u>Scaling</u>



$t(\ell) \sim \ell^2/D$

After $t(\ell)$ only one A left $\Rightarrow$

$$\rho = \frac{1}{\ell} \sim \frac{1}{\sqrt{Dt}}$$

[Also $A + B \rightarrow \phi$]

<u>Reaction-Diffusion eqs.</u>

$\rho \rightarrow \rho(\vec{x}, t)$

$$\frac{\partial}{\partial t}\rho = \mathcal{R}(\{\rho(\vec{x},t)\}) + D\Delta\rho$$

mean-field　　　diffusion

Of~~ten~~ fails (can't manage both a cell <u>large</u> enough for ρ con<u>tinuous</u> yet <u>small</u> enough for <u>MF reaction rate</u>
