Reaction–Diffusion Models in One Dimension

2. "A Gift from the Gods;" $A+A \to A$ and the method of Empty Intervals

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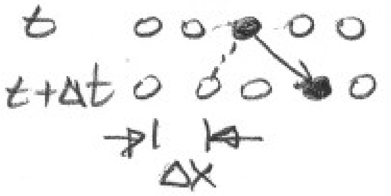
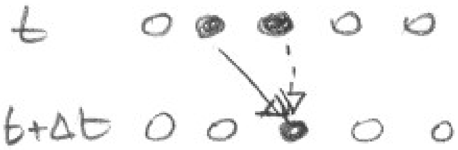
The model:

diffusion



[rate $\frac{D}{(\Delta x)^2}$ to each side]

coalescence



[**]

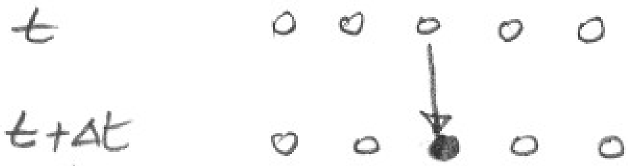
birth

[$\frac{\nu}{2\Delta x}$ to each side]

* updating is not parallel

** Coalescence is assumed also for input and birth processes. Rate is the rate of the parent process.

input



[$R\Delta x$]

Empty intervals:

$E_n(t) \equiv$ prob. that n consecutive sites are empty at time t

$$c(t) = \frac{1-E_1(t)}{\Delta x} \qquad [1-E_1 \equiv \text{Prob}(\bullet)]$$

$$\text{Prob.}\left(\overset{1}{\circ}\overset{2}{\circ}\cdots\overset{n}{\circ}\overset{n+1}{\bullet}\right) \equiv x$$

$\overset{1}{\circ}\overset{2}{\circ}\cdots\overset{n}{\circ}\overset{n+1}{\bullet}$	x
$\circ\circ\cdots\circ\circ$	E_{n+1}
$\circ\circ\cdots\circ$	E_n

$$\Rightarrow x + E_{n+1} = E_n \Rightarrow \boxed{x = E_n - E_{n+1}}$$

Consider now $\Delta E_n(t)$ during a time Δt:

* E_n does not change through diffusion inside n-gap: $\overset{1}{\circ}\circ\circ\bullet\overset{n}{\circ}$

but changes throug diffusion into or out of the gap $\overset{1}{\circ}\overset{2}{\circ}\circ\cdots\overset{n}{\circ}\bullet$; $\circ\circ\cdots\circ\bullet\circ$

$$(\Delta E_n)_{\text{diff.}} = \frac{2D}{(\Delta x)^2}\Delta t\left[-(E_n - E_{n+1}) + (E_{n-1} - E_n)\right]$$

$$= \frac{2D}{(\Delta x)^2}\Delta t\left[E_{n-1} - 2E_n + E_{n+1}\right]$$

note that we do not care about the state of this site!

* E_n does <u>not</u> change due to birth <u>inside</u> n-gap 

,

but changes if birth occurs at an outer edge:

$$(\Delta E_n)_{\text{birth}} = -\frac{v}{\Delta x}\Delta t\,(E_n - E_{n+1})$$

* $(\Delta E_n)_{\text{input}} = -(Rn\Delta x)\Delta t\, E_n$

$$\frac{\Delta E_n}{\Delta t} = \frac{2D}{(\Delta x)^2}\left[E_{n-1} - 2E_n + E_{n+1}\right] - \frac{v}{\Delta x}(E_n - E_{n+1}) - Rn\Delta x E_n$$

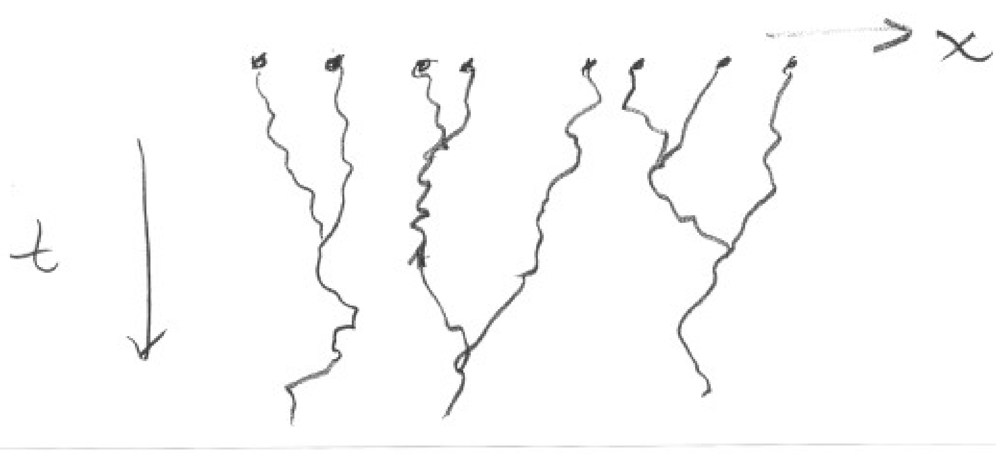
Continuum limit: $\Delta x \to 0$, $\Delta t \to 0$; $n\Delta x \equiv x$

$$E_n(t) \to E(x,t)$$

$$E_{n-1} = E(x-\Delta x, t) = -(\Delta x)\frac{\partial}{\partial x}E(x,t) + E(x,t)$$

$$\Rightarrow \boxed{\frac{\partial E}{\partial t} = 2D\frac{\partial^2}{\partial x^2}E + v\frac{\partial}{\partial x}E - RxE}$$

<u>Simple coalescence</u>: Assume $v=0$, $R=0$



Exercise: Initial random condition

Suppose a fraction p of the sites are occupied, initially $\left(c(0) = \frac{p}{\Delta x} \equiv c_0\right)$
Compute E_n and then $E(x,0)$, taking the appropriate limit. $\left[E(x,0) = e^{-c_0 x}\right]$

Gap pdf

$$y_n \equiv \text{prob}\,(\bullet \overset{1\,2\,\cdots\,n}{\circ\circ\cdots\circ} \bullet)$$

	$1\ 2 \cdots n$		
$\bullet$	$\circ\circ\cdots\circ$	$\bullet$	y
$\bullet$	$\circ\circ\cdots\circ$	$\circ$	$E_{n+1} - E_{n+2}$
$\circ$	$\circ\circ\cdots\circ$	$\bullet$	$E_{n+1} - E_{n+2}$
$\circ$	$\circ\circ\cdots\circ$	$\circ$	E_{n+2}
$\times$	$\circ\circ\cdots\circ$	$\times$	E_n

then $y_n = E_n - E_{n+2} - 2(E_{n+1} - E_{n+2})$

or $\boxed{y_n = E_n - 2E_{n+1} + E_{n+2}}$

Exercise: Let $p(x,t)$ be the conditional prob. that the gap from a given particle to the next is x (in the continuous limit). Show that

$$c(t)\,p(x,t) = \frac{\partial^2 E}{\partial x^2}$$

Boundary condition

We have no equation for ΔE_1 (E_0 is not defined).

$\Delta E_1 = -\Delta(1-E_1)$ is related to the rate of the coalescence process: t ●● → $t+\Delta t$ ●○

$$\Delta E_1 = \frac{D}{(\Delta x)^2}\Delta t\, \mathrm{prob}(●●)$$
$$= \frac{D}{\Delta x^2}\Delta t(1-2E_1+E_2)$$

●●	z
○●	$E_1 - E_2$
●○	$E_1 - E_2$
○○	E_2
××	1

$z = 1-2E_1+E_2$

Comparing with

$$\Delta E_n = \frac{D}{(\Delta x)^2}\Delta t\,(E_{n-1} - 2E_n + E_{n+1})$$ we conclude

that $\begin{cases} E_0 = 1 \\ E(0,t) = 1 \end{cases} \Rightarrow c(t) = \frac{1-E_1}{\Delta x} = \frac{E_0 - E_1}{\Delta x} \to -\frac{\partial E}{\partial x}\Big|_{x=0}$

$\boxed{\text{Exercise: same BC even when } v, R \neq 0}$

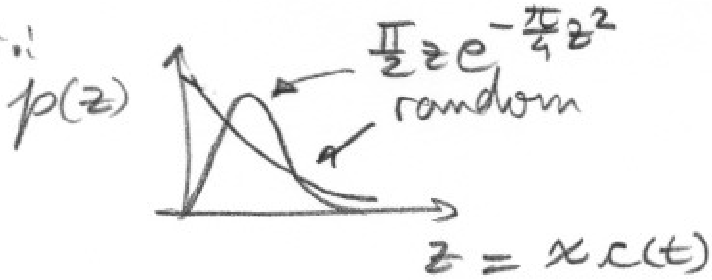
To sum up:

$$\left.\begin{aligned} \frac{\partial E(x,t)}{\partial t} &= 2D\frac{\partial^2}{\partial x^2}E(x,t) \\ \text{IC:}\quad E(x,0) &= e^{-c_0 x} \\ \text{BC:}\quad E(0,t) &= 1 \end{aligned}\right\} \Rightarrow \begin{aligned} c(t) &= -\frac{\partial E}{\partial x}\Big|_{x=0} \\ p(x,t) &= \frac{\partial^2 E}{\partial x^2}\Big/ c(t) \end{aligned}$$

Exercise: solve and work out long-time asymptotic limit of $c(t)$, $p(x,t)$ [Ans: $c(t) \to \frac{1}{\sqrt{8\pi D t}}$

$p(x,t) \to \frac{x}{4Dt}e^{-x^2/8Dt}$]

Gap dist.:



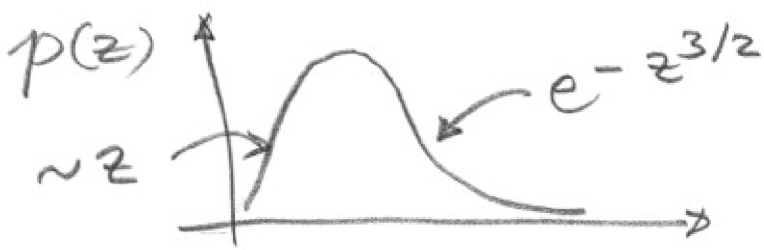
Input $\quad \frac{\partial}{\partial t} E = 2D \frac{\partial^2}{\partial x^2} E - x R E$

steady-state is Airy's eq:

$$E_{xx} = \frac{R}{2D} x E$$

$$\Rightarrow E = Ai\left(\left(\tfrac{R}{2D}\right)^{1/3} x\right) / Ai(0)$$

$$c_s \propto \left(\tfrac{R}{2D}\right)^{1/3}$$



Birth $\quad$ Full equilibrium $\quad A + A \rightleftharpoons A$

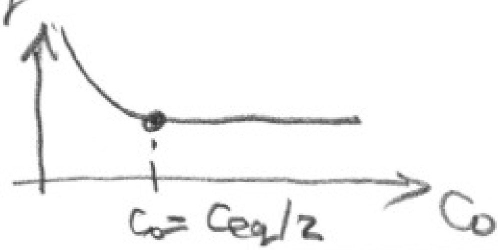
$$\frac{\partial}{\partial t} E = 2D \frac{\partial^2}{\partial x^2} E + v \frac{\partial}{\partial x} E \Rightarrow E_{eq} = e^{-vx/2D}$$

$$c_{eq} = \frac{v}{2D}$$

Approach to eq.

$$p_{eq} = \frac{v}{2D} e^{-vx/2D}$$

$$c(t) - c_{eq} \sim e^{-t/\tau}$$



$\boxed{\text{dynamical phase transition}}$