Reaction-Diffusion Models in One Dimension

3. $A+A\to\phi$ and Advanced Applications of Empty Intervals

Inhomogeneous system of $A+A\to A$

Replace $E_n(t)$ with $E_{n,m}(t) = \text{Prob}(\underset{n}{\circ}\,\underset{n+1}{\circ}\cdots\underset{m}{\circ})$

In continuum limit $E_{n,m}(t) \to E(x,y,t)$, $x = n\Delta x$, $y = m\Delta x$

(Guided!)
Exercise

(a) show $\dfrac{\partial E(x,y,t)}{\partial t} = D\left(\dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2}\right) E(x,y,t)$

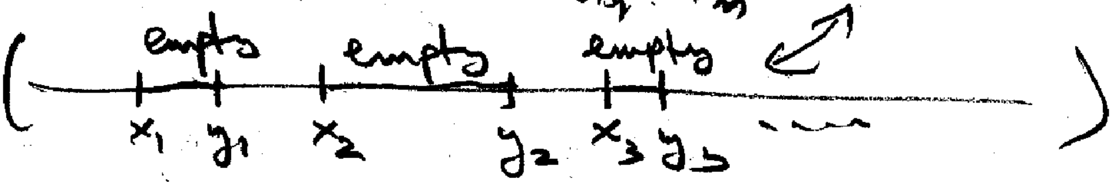
(b) with BCs: $\lim\limits_{\substack{x\nearrow y \\ \text{or } y\searrow x}} E(x,y,t) = 1$

(c) $\rho(x,t) = -\dfrac{\partial}{\partial y} E(x,y,t)\Big|_{y=x} = +\dfrac{\partial}{\partial x} E(x,y,t)\Big|_{y=x}$

(d) $p(x,y,t) = \rho(x,t)^{-1}\dfrac{\partial^2}{\partial x\,\partial y} E(x,y,t)$ Note asymmetry and provide meaning

Also, n-point correlation function

$$\rho_n(x_1,x_2,\ldots,x_n,t) = \frac{\partial^n}{\partial x_1\cdots\partial x_n} E_n(x_1,y_1,x_2,y_2,\ldots,x_n,y_n,t)\Bigg|_{\substack{y_1=x_1,\\ y_2=x_2,\\ \vdots \\ y_n=x_n}}$$

Prob()

Supplement to Lecture 2

Scaling solution of A+A→A

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

Assume scaling: as $t\to\infty$ $E(x,t) \equiv f(xc) \equiv f(z)$

Note that $c = -\frac{\partial E}{\partial x}\Big|_{x=0} = -cf'(0) \Rightarrow \boxed{f'(0)=-1}$

Substituting...

$$\frac{\partial}{\partial t} f(z) = 2D\frac{\partial^2}{\partial x^2} f(z) \Rightarrow x\dot{c} f' = 2Dc^2 f'' \quad / x \text{ times}$$

$$\underbrace{(xc)}_{z}\,\dot{c} f' = 2Dc^3 f''$$

to be consistent with scaling we need

$$\frac{\dot{c}}{2Dc^3} = -A \quad =(\text{const}) \Rightarrow c \sim 1/\sqrt{4ADt} \ \ldots \text{ but wait.}$$

$$-Az = \frac{f''}{f'} \Rightarrow f' = \beta e^{-Az^2/2} = -e^{-Az^2/2}$$

$\beta = -1$ since $f'(0)=-1$

But then $E = f = 1 - \int_0^z f(y)\,dy = 1 - \int_0^z e^{-Ay^2/2}\,dy$

since $E(0)=1$

But $E(\infty,t)=0 \Rightarrow \int_0^\infty e^{-Ay^2/2}\,dy = \sqrt{\frac{2\pi}{A}} = 1 \Rightarrow \boxed{A=2\pi}$

Example: 2-point correlations for $A+A\to\emptyset$

$$\frac{\partial}{\partial t} E_2(x_1,y_1,x_2,y_2,t) = D\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial y_1^2}+\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial y_2^2}\right) E_2$$

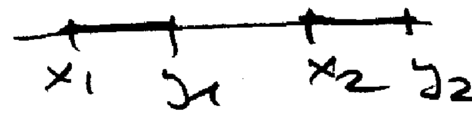
BCs:

$$\lim_{\substack{x_1 \nearrow y_1 \\ \text{or } y_1 \searrow x_1}} E_2(x_1,y_1,x_2,y_2,t) = E_1(x_2,y_2,t)$$

needs its own equation

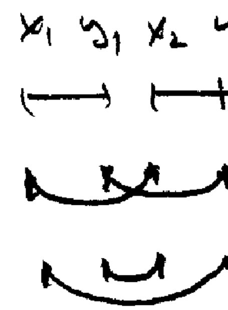
$$\lim_{\substack{y_1 \nearrow x_2 \\ \text{or } x_2 \searrow y_1}} E_2(x_1,y_1,x_2,y_2,t) = E_1(x_1,y_2,t)$$

etc...



Solution (drop t, for brevity)

$$\begin{aligned} E_2(x_1,y_1,x_2,y_2) &= E(x_1,y_1)E(x_2,y_2) \\ &\quad - E(x_1,x_2)E(y_1,y_2) \\ &\quad + E(x_1,y_2)E(y_1,x_2) \end{aligned}$$



check!

With some more effort (☺) one obtains the full solution for the full hierarchy:

$$E_n(x_1,y_1,x_2,y_2,\dots,x_n,y_n) = \sum_{p=1}^{(2n-1)!!} \sigma_p E(z_{1p},z_{2p})E(z_{3p},z_{4p}) \cdots E(z_{2n-1,p},z_{2n,p})$$

Also recursion form

$z_{1p}\dots z_{2np}$ is an ordered permutation of $x_1,\dots,y_n$

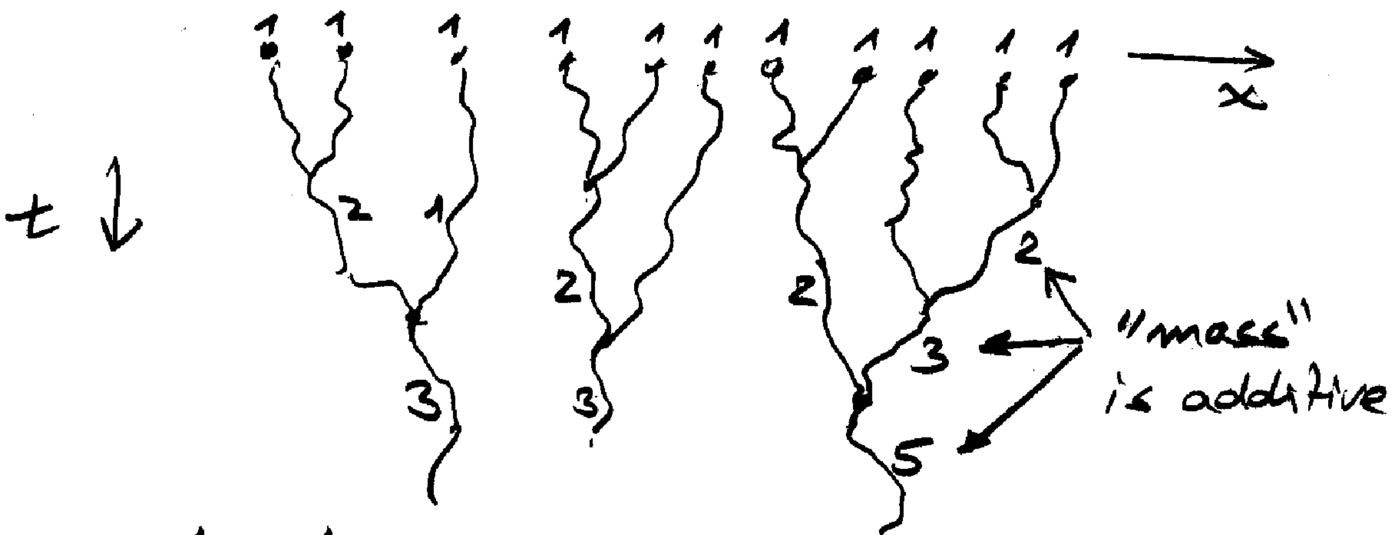
$z_{1p}<z_{2p}$, $z_{3p}<z_{4p}$, ..., $z_{2n-1,p}<z_{2n,p}$

and $z_{1p}<z_{3p}<z_{5p}<\dots<z_{2n,p}$

$\sigma_p = \pm 1$ for even/odd permutations

Another good example is "Fisher fronts" (will detail the problem in lecture 4)

Annihilation & Coalescence



$$A_i + A_j \to A_{i+j}$$

(a) Ignore mass $\Rightarrow$ $A + A \to A$

(b) Observe only particles with odd mass $\Rightarrow$ $A + A \to \phi$ ← even mass $\left(\begin{array}{l} \text{odd+odd} \to e \\ e+e \to e \\ e+o \to o \end{array}\right)$

* Mass distribution interesting problem on its own right (Takayasu)

Odd/Even (Parity) - Intervals

$G_n(t) \equiv$ prob. that n-sites contain <u>even</u> number of particles $(0, 2, 4, \dots)$ | $p = 1 - G_1$

We need:

$F_n(t) \equiv \text{prob}\big(\underbrace{\overset{\text{even}}{\cdots\cdots}}_{n}\ \underset{n+1}{\bullet}\big)$

Notation:

$\underbrace{\overset{\text{even}}{\cdots\cdots}}_{n} \rightarrow$ empty bar of length n

$\underbrace{\overset{\text{odd}}{\cdots\cdots}}_{n} \rightarrow$ hatched bar of length n

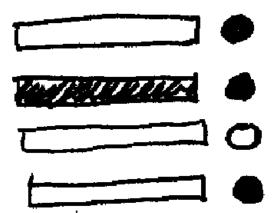
single site: $\circ$ empty, $\bullet$ occupied

$1 \quad\quad n$

F_n

G_{n+1}

F_n



$\}\ 1 - G_1 \quad (\bullet)$

$\}\ G_n$ (empty bar)

$$2F_n + G_{n+1} = 1 - G_1 + G_n$$

$$\text{or} \quad F_n = \frac{1-G_1}{2} + \frac{G_n - G_{n+1}}{2}$$

$H_n \equiv \text{prob}\big(\underbrace{\text{hatched bar}}_{n}\ \bullet\big) \qquad H_n + F_n = 1 - G_1$

$$\Rightarrow \quad H_n = \frac{1-G_1}{2} - \frac{G_n - G_{n+1}}{2}$$

$\Rightarrow$ can do everything with the G_n's alone!

Example

$n-1 \qquad n$

$$\left(\Delta G_n\right)_{\text{diff.}} = \frac{2D}{(\Delta x)^2}\Delta t\left[F_{n-1} - H_{n-1} + H_n - F_n\right]$$

$n-1 \qquad n$

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

Applications

* Various types of input: → A - - - A pairs
  → A (single)
  → BRW

* q-state Potts model ($T \to 0$, Glauber dynamics)

q tipes of states: kinks A_{ij} between states of type iii & jjj

reactions between kinks:

(1) $A_{ij} + A_{ji} \to \emptyset$

(2) $A_{ij} + A_{jk} \to A_{ik}$

If $q=2$ (2) does not happen ($A+A \to \emptyset$)

If $q \to \infty$ (1) does (almost) never happen ($A+A \to A$)

Let G_n denote interval containing a total number of indices (eg A_{ij}) that is even
pairs of kink

⇒ Exactly same eq. for G_n as before!

Only change is in initial cond:

If random, $G_n(0) = \frac{1}{q}$

$$\Rightarrow c_q(t) = \frac{q-1}{q} c_{coal}(t)$$

* n-point correlation functions for annihilation:

$$F_n(x_1,y_1,x_2,y_2,\dots,x_n,y_n) = \mathrm{Prob}(\#\text{ of particles in } \bigcup_{i=1}^{n}[x_i,y_i] \text{ is even})$$

$$H_n(\underbrace{x_1,y_1}_{\text{even}}, \underbrace{\overline{x_2,y_2}}_{\text{odd}}, \dots, \underbrace{\overline{x_i,y_i}}_{\text{odd}}, \dots, \underbrace{x_j,y_j}_{\text{even}})$$
$\equiv$ Prob(even odd odd ... even

eg. $F_2(x_1,y_1,x_2,y_2) = H_2(x_1,y_1,x_2,y_2) + H_2(\overline{x_1,y_1},\overline{x_2,y_2})$

In general F_n is the sum of 2^n H_n's, and since $\rho = \frac{\partial}{\partial x} G(x,y)\Big|_{y=x}$

$$\Rightarrow \rho_n^{\text{anni}}(x_1,x_2,\dots,x_n,t) = \frac{1}{2^n}\frac{\partial^2}{\partial x_1\partial x_2\cdots\partial x_n}F_n\Big|_{\vec{y}=\vec{x}}$$

$$\Rightarrow \boxed{\rho_n^{\text{anni}} = \frac{1}{2^n}\rho_n^{\text{coal}}} \ !$$

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* $\omega_n \Leftrightarrow \rho_n$ hierarchies

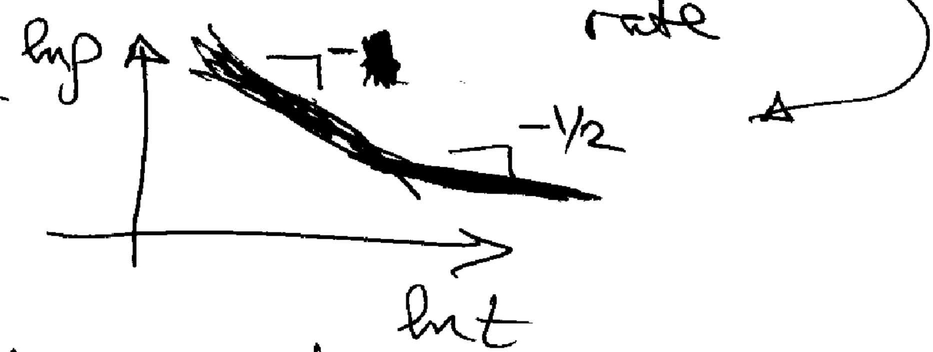
Approximations

We can't express $\text{Prob}(\underbrace{\circ,\circ,\dots}_{n},\underset{n+1}{\bullet},\underset{n+2}{\bullet})$
with the E_n, but if we could, we could analyze lots more interesting situations, such as

(1) $3A \to A$

(2) $A + A \to A$ but ~~finite~~ finite reaction rate

Crossover



$\Rightarrow$ Approximate a la Kirkwood:

$$\text{Prob}(\underbrace{\circ\circ\circ\circ}_{n}\bullet\bullet) \simeq \frac{\text{Prob}(\underbrace{\circ\circ\cdots\circ}_{n}\bullet)\,\text{Prob}(\bullet\bullet)}{\text{Prob}(\bullet)}$$

Exact in early time regime (no initial correlations)

And late times: ~~Prob~~ reaction rate "renormalizes" to infinite ...