# Kinetic models in statistical physics 

B. Kahng<br>Seoul National University<br>bkahng@snu.ac.kr

The 18th KIAS-APCTP Winter School on Statistical Physics Jan 11,2021 - Jan 15,2021

## Contents

(1) Overview
(2) References
(3) Diffusion, Random Walks on fractal structure

- Random walks
- Gaussian model
- Self-avoiding walks and $n$-vector cubic model
(4) Kinectics of reaction process
- Single-species annihilation/coalescence
- Two-species annihilation
- Two-species annihilation on fractal structure
- Two species annihilation on SF networks
(5) Aggregation


## Contents

## (1) Overview

(2) References
(3) Diffusion, Random Walks on fractal structure

- Random walks
- Gaussian model
- Self-avoiding walks and $n$-vector cubic model
(4) Kinectics of reaction process
- Single-species annihilation/coalescence
- Two-species annihilation
- Two-species annihilation on fractal structure
- Two species annihilation on SF networks
(5) Aggregation


## Where are we now?

## Q1 통계물리학에서는 어떤 주제를 연구했었는가?

Q2 최근에는 어떤 주제를 연구하는가?

## Q3 어떤 중요한 연구 문제가 남아있는가?

## Contents

## (1) Overview

## (2) References

(3) Diffusion, Random Walks on fractal structure

- Random walks
- Gaussian model
- Self-avoiding walks and $n$-vector cubic model
(4) Kinectics of reaction process
- Single-species annihilation/coalescence
- Two-species annihilation
- Two-species annihilation on fractal structure
- Two species annihilation on SF networks
(5) Aggregation


## References

- Pavel L Krapivsky, Sidney Redner, and Eli Ben-Naim. A Kinetic View of Statistical Physics (Cambridge University Press, 2010).
- 김두철, 프랙탈 격자계의 물리적 성질 in 통계물리학의 발전: 용봉 조순탁교수 환갑을 기념하여 (비매품, 1985년)
- D. Kim 'Random walks and Gaussian Model on Fractal Lattices," JKPS 17, 271, (1984).
- D. Kim and B. Kahng, "Comments on the self-avoiding walks on finitely ramified fractals," PRA 31, 1193 (1985).
- C.-K. Yun, B. Kahng, and D. Kim, "Annihilation of two-species reaction-diffusion processes on fractal scale-free networks," New. J. Phys. 11, 063025 (2009).
- D. Kim, 연구노트 091102
- 강병남, 복잡계 네트워크 과학, (민음사, 2010).


## Contents

## (1) Overview

(2) References
(3) Diffusion, Random Walks on fractal structure

- Random walks
- Gaussian model
- Self-avoiding walks and $n$-vector cubic model
(4) Kinectics of reaction process
- Single-species annihilation/coalescence
- Two-species annihilation
- Two-species annihilation on fractal structure
- Two species annihilation on SF networks
(3) Aggregation


## Random walks

(I) $P_{n}(x)$ is the occupation probability at site $x$ at time step $n$.

$$
P_{n}(x)=p P_{n-1}(x-1)+q P_{n-1}(x+1)
$$

These random walks may be understood as a binomial process, $\prod_{n}(r)$ that the walk takes $r$ steps to the right and $n-r$ steps to the left. $\prod_{n}(r)=\binom{n}{r} p^{r} q^{n-r}$. Using the stirling's approximation and $x=2 r-n$, $n!\sim \sqrt{2 \pi n}\left(\frac{n}{e}\right)^{n}$

$$
\begin{aligned}
P_{n}(x)=\prod_{n}[(x+n) / 2] & =\frac{1}{\sqrt{2 \pi n p q}} e^{-[x-n(p-q)]^{2} / 2 n p q} \\
& =\frac{1}{\sqrt{2 \pi n \sigma^{2}}} e^{-[x-n\langle x\rangle]^{2} / 2 n \sigma^{2}} \\
& =\frac{1}{\sqrt{4 \pi D n}} e^{-[x-n\langle x\rangle]^{2} / 4 D n} \quad\left\langle x^{2}\right\rangle=2 D t
\end{aligned}
$$

## Random walks

(II) The master equation:
( $n$ is a position)

$$
\frac{\partial P_{n}}{\partial t}=P_{n+1}-2 P_{n}+P_{n-1} . \text { Using } P(k, t)=\sum_{n=-\infty}^{\infty} P_{n}(t) e^{i k n}
$$

$$
\frac{\partial P(k, t)}{\partial t}=2(\cos k-1) P(k, t) \Rightarrow P(k, t)=e^{2(\cos k-1) t}
$$

$$
e^{x \operatorname{cosk}}=\sum_{n=-\infty}^{\infty} e^{i k n} I_{n}(x) \rightarrow P_{n}(t)=I_{n}(2 t) e^{-2 t} \xrightarrow{t \rightarrow \infty} \frac{1}{\sqrt{4 \pi t}} e^{-n^{2} / 4 t}
$$

Modified Bessel function:
$I_{n}(x)=\frac{1}{2 \pi i} \oint e^{(x / 2)(t+1 / t)} t^{-n-1} d t$

## Random walks

## Transition matrix

$P_{i, j}(n)$ : Probability that a random walker starting from site $i$ is at site $j$ at time step $n$.

$$
\begin{aligned}
P_{i, j}(n) & =\sum_{j_{1}} W_{j_{1}, j} P_{i, j_{1}}(n-1)=\sum_{j_{1}} W_{j_{1}, j} \sum_{j_{2}} W_{j_{2}, j_{1}} P_{i, j_{2}}(n-2) \\
& =\cdots=\sum_{j_{1}} \sum_{j_{2}} \cdots \sum_{l} W_{j_{1}, j} W_{j_{2}, j_{1}} \cdots W_{j_{n-1} \rightarrow j_{n-2}} W_{i, j_{n-1}} \\
& =\left(W^{n}\right)_{i, j}
\end{aligned}
$$

The generating function (g-function) of $P_{i \rightarrow j}(n)$ :

$$
\begin{aligned}
\mathcal{P}_{i, j}(s) & \equiv \sum_{n=0}^{\infty} P_{i, j}(n) s^{n}=\sum_{n=0}^{\infty}\left(W^{n}\right)_{i, j} s^{n}=\left(\frac{1}{I-s W}\right)_{i, j} \\
& =\left(\frac{1}{(1-s) I+s w V}\right)_{i, j}
\end{aligned}
$$

In Euclidean lattice

$$
W_{i, j}= \begin{cases}\frac{1}{2 d} & (i, j) \text { is n.n } \\ 0 & \text { otherwise }\end{cases}
$$

Generally,

$$
W_{i, j}= \begin{cases}w & (i, j) \text { is n.n } \\ 1-z_{i} w & i=j \\ 0 & \text { otherwise }\end{cases}
$$

$z_{i}$ : coordination number of site $i$ s.t.

$$
1-z_{i} w \geq 0
$$

$$
\begin{gathered}
\text { Laplacian matrix } V_{i, j} \equiv \begin{cases}-1 & (i, j) \text { is n.n } \\
z_{i} & i=j \\
0 & \text { otherwise }\end{cases} \\
\Rightarrow W=I-w V
\end{gathered}
$$

## Random walks

Return to the origin
$P_{o}(n)$ : Probability to return to the origin (any starting site $i$ ) after time $n$

$$
P_{o}(n)=\frac{1}{N} \sum_{i=1}^{N} P_{i, i}(n)
$$

The g-function of $P_{o}(n)$ :

$$
\begin{aligned}
\mathcal{P}_{o}(s) & \equiv \sum_{n=0}^{\infty} P_{o}(n) s^{n}=\frac{1}{N} \sum_{i}\left(\frac{1}{(1-s) I+s w V}\right)_{i, i} \\
& =\frac{1}{N} \sum_{\ell} \frac{1}{(1-s)+s w \lambda_{\ell}} \\
& =\int_{0}^{\infty} \frac{\rho_{s}(\lambda) d \lambda}{1-s(1-w \lambda)}=\sum_{n=0} \int_{0}^{\infty} s^{n}(1-w \lambda)^{n} \rho_{s}(\lambda) d \lambda
\end{aligned}
$$

$$
\Rightarrow P_{o}(n)=\int_{0}^{\infty}(1-w \lambda)^{n} \rho_{s}(\lambda) d \lambda \approx \int_{0}^{\infty} e^{-n w \lambda} \rho_{s}(\lambda) d \lambda
$$

where $\rho_{s}(\lambda)$ is the spectral density of Laplacian matrix $V$.

## P1) Show the following:

Consider a harmonic motion: $m \frac{d^{2} x_{i}}{d t^{2}}=-k \sum_{j \in \text { n.n. of } i}\left(x_{i}-x_{j}\right)$ $\lambda x_{i}=\sum_{j} V_{i, j} x_{j}$
Then the eigenvalue $\lambda \sim \omega^{2}$, and the spectral density is $\rho_{s}(\lambda) \sim \lambda^{\frac{d_{s}}{2}-1}$ ( $d_{s}$ : spectral dimension)

P2) Show the following:
$\Rightarrow P_{o}(n) \sim n^{-d_{s} / 2} \Rightarrow \mathcal{P}_{o}(s) \sim(1-s)^{\frac{d s}{2}-1} \rightarrow$ singular when $d_{s}<2$ as $s \rightarrow 1$.

## Mean distance

$R_{i j}$ is the distance from site $i$ to $j$
Mean distance after $n$ time steps: ( $d_{w}$ : random-walk dimension)

$$
\left\langle R_{n}^{2}\right\rangle=\frac{1}{N} \sum_{i} \sum_{j} R_{i j}^{2} P_{i, j}(n) \sim n^{2 / d_{w}}
$$

$R^{2}(s)=\sum_{n=0}^{\infty}\left\langle R_{n}^{2}\right\rangle s^{n} \sim \sum_{n} n^{2 / d_{w}} s^{n} \sim$
$\left\langle R_{n}^{2}\right\rangle=2 D n$ in Euclidean lattice. $D$ is diffusion constant. $d_{w}=2$.
The number of sites within radius $R$ is $M \sim R^{d_{f}} \sim n^{d_{f} / d_{w}}$.
The prob. to return to the origin: $P_{o}(n) \sim \frac{1}{M} \sim n^{-d_{f} / d_{w}} \sim n^{-d_{s} / 2}$

$$
d_{w}=\frac{2 d_{f}}{d_{s}}
$$

$\rightarrow$ For $d_{s} \leq 2$, a RW surely returns to the origin, so that the walk is recurrent.
$\rightarrow$ For $d_{s}>2$, RW never returns, and the walk is transient.

## Laplacian transform and Generating function

For $f(t) \sim t^{-\mu}(t \gg 1$ and $\mu<1)$, the Laplace transform is given as follows:

$$
\begin{aligned}
f(s)= & \int_{0}^{\infty} t^{-\mu} e^{-s t} d t \\
= & s^{\mu-1} \int_{0}^{\infty} x^{-\mu} e^{-x} d x=\Gamma(1-\mu) s^{\mu-1} \\
& \Gamma(z)=\int_{0}^{\infty} x^{z-1} e^{-x} d x
\end{aligned}
$$

$$
\begin{aligned}
R^{2}(s) & \sim \sum_{n} n^{2 / d_{w}} s^{n} \sim \sum_{n} n^{2 / d_{w}} e^{n \ln s} \quad \text { for } \quad 0<s<1 \\
& \sim \sum_{n} n^{2 / d_{w}} e^{-n(1-s)} \sim \Gamma\left(2 / d_{w}+1\right)(1-s)^{-\left(2 / d_{w}+1\right)}
\end{aligned}
$$

## First-passage properties

$P(r, t)$ is the occupation prob. of a RW.
$F(r, t)$ is the prob. for a RW to first reach $r$ at $t$.

$$
P(r, t)=\int_{0}^{t} F\left(r, t^{\prime}\right) P\left(0, t-t^{\prime}\right) d t^{\prime}+\delta_{r, 0} \delta(0)
$$

Laplace transforms: $F_{L}(r, s)=\frac{P_{L}(r, s)-\delta_{r, 0}}{P_{L}(0, s)}$
The eventual return probability to the origin: $\mathcal{R}=F_{L}(0,0)=\int_{0}^{\infty} F(0, t) d t$ If $\mathcal{R}=1$, the walk is recurrent, and otherwise, it is transient.
Using $P(t) \simeq \frac{1}{(4 \pi t)^{d / 2}}$ as $t \rightarrow \infty$,
P3) Show that $F(t) \simeq \frac{1}{\sqrt{\pi}} \frac{1}{t^{3 / 2}}$ in $1 \mathrm{~d} ; F(t) \simeq \frac{4 \pi}{t(\ln t)^{2}}$ in 2 d ; and
$F(t) \simeq \frac{(1-\mathcal{R})^{2}}{8 \pi^{3 / 2}} \frac{1}{t^{3 / 2}}$ in 3 d . Find $\mathcal{R}$ in 3 d .

## Vicious random walks

When two random walks meet, they mutually annihilate. What is their survival prob.?
$\rightarrow$ Consider two RWers starting from $x_{1}$ and $x_{2}$. Their relative position is $y=x_{2}-x_{1}$ for $x_{2}>x_{1}$.

$$
c(y, t)=\frac{1}{\sqrt{8 \pi D t}}\left[e^{-\left(y-y_{0}\right)^{2} / 8 D t}-e^{-\left(y+y_{0}\right)^{2} / 8 D t}\right]
$$

P4) show that $F(t) \sim \frac{y_{0}}{\sqrt{8 \pi D t^{3}}} e^{-y_{0}^{2} / 8 D t} \sim t^{-3 / 2}$
The survival probability $S(t)=1-\frac{2}{\sqrt{\pi}} \int_{y_{0} / \sqrt{8 D t}}^{\infty} e^{-u^{2}} d u \rightarrow \frac{y_{0}}{\sqrt{2 \pi D t}}$

## Gaussian model: a spin model of RWs

$$
-\beta H=\beta \sum_{<i, j>} W_{i, j} \phi_{i} \phi_{j}+\sum_{i} h_{i} \phi_{i},
$$

$\phi_{i}$ is a spin continuous variable at site $i$ in the range $[-\infty, \infty]$ with weight $e^{-\phi_{i}^{2}}$. The partition function is given as

$$
\begin{aligned}
Z & =\int[d \phi] e^{-\sum_{i} \phi_{i}^{2}+\beta \sum_{<i j>} W_{i j} \phi_{i} \phi_{j}+\sum_{i} h_{i} \phi_{i}} \\
& =\Pi_{l}\left[\frac{\pi}{1-\beta \lambda_{l}}\right]^{\frac{1}{2}} \exp \left[\left(\sum_{i} h_{i} a_{i l}\right)^{2} / 4\left(1-\beta \lambda_{l}\right)\right]
\end{aligned}
$$

Internal energy: With $h_{i}=0$,

$$
\begin{aligned}
u & =-\frac{1}{N} \frac{\partial}{\partial \beta}(\ln Z)= \\
& =\frac{1}{2 \beta}\left(1-\frac{1}{N} \sum_{i} \frac{1}{I-\beta W}\right)_{i i}
\end{aligned}
$$

because $\sum_{j} W_{i, j}=1, a_{i, 0}=\frac{1}{\sqrt{N}}$ and $\lambda_{0}=1 . \sum_{l} a_{i l} a_{j l}=\delta_{i, j}$

$$
\begin{gathered}
u \sim\left(1-\frac{\beta}{\beta_{c}}\right)^{1-\alpha_{g}} \Leftrightarrow \mathcal{P}_{o}(s) \sim(1-s)^{\frac{d_{s}}{2}-1} \\
1-\alpha_{g}=\frac{d_{s}}{2}-1 \Rightarrow 2-\alpha_{g}=\frac{d_{s}}{2}=\frac{d_{f}}{d_{w}}=d_{f} \nu_{g}
\end{gathered}
$$

Correlation function

$$
\begin{aligned}
\Gamma_{i j}=\frac{\partial^{2} \ln Z}{\partial h_{i} \partial h_{j}} & =\left\langle\phi_{i} \phi_{j}\right\rangle-\left\langle\phi_{i}\right\rangle\left\langle\phi_{j}\right\rangle \\
& =\frac{1}{2} \sum_{l} \frac{a_{i l} a_{j l}}{1-\beta \lambda_{l}}=\frac{1}{2}\left(\frac{1}{I-\beta W}\right)_{i, j} \Leftrightarrow \mathcal{P}_{i \rightarrow j}(\beta)
\end{aligned}
$$

Susceptibility

$$
\chi=\frac{1}{N} \sum_{i, j} \Gamma_{i, j}=\frac{1}{2 N} \sum_{i, j, l} \frac{a_{i l} a_{j l}}{1-\beta \lambda_{l}}=
$$

because $\sum_{j} W_{i, j}=1, a_{i, 0}=\frac{1}{\sqrt{N}}$ and $\lambda_{0}=1 . \sum_{l} a_{i l} a_{j l}=\delta_{i, j} \gamma_{g}=1$

Correlation length

$$
\xi^{2}=\sum_{i j} R_{i j}^{2} \Gamma_{i j} / \sum_{i j} \Gamma_{i j} .
$$

Mean distance $\left\langle R_{n}^{2}\right\rangle$, and its g-function $R^{2}(s)=\sum_{n=0}^{\infty}\left\langle R_{n}^{2}\right\rangle z^{n}$

$$
\begin{gathered}
R^{2}(s)=\xi^{2}(s) \chi(s) \sim(1-s)^{-2 \nu_{g}-\gamma_{g}} \sim(1-s)^{-2 \nu_{g}-1} \\
R_{n}^{2} \sim n^{2 \nu_{g}} \quad\left(\nu_{g}=1 / d_{w}\right)
\end{gathered}
$$

P5) Consider a Sierpinski gasket. i) Obtain the fractal dimension. Consider random walks on an infinite Sierpinski gasket. ii) Obtain the spectral dimension and random walk dimension.

## Sierpinski Gasket and Self-avoiding walks



## Self-avoiding walks

A model for solvent or polymer configuration. Non-markovian process.
$\Gamma_{i, j}(n)$ is the number of ways for a SAWer starting from site $i$ to reach site $j$ after $n$ steps.

Its generating function: $\Gamma_{i, j}(s)=\sum_{s=0}^{\infty} \Gamma_{i, j}(n) s^{n}$
$N_{i}(n)$ is the number of ways for the SAWer to reach any site after $n$ steps: $N_{i}(n)=\sum_{j} \Gamma_{i, j}(n)$
$N(n)=\frac{1}{N} \sum_{i} N_{i}(n)$ and $N(s)=\sum_{n} N(n) s^{n}$.
If $N(n) \sim n^{\gamma-1} \mu^{n}$, then $N(s) \sim(1-\mu s)^{-\gamma}$, where $\mu=1 / s_{c}$.
$\left\langle R^{2}(n)\right\rangle=\sum_{i, j} R_{i j}^{2} \Gamma_{i j} / \sum_{i, j} \Gamma_{i j} \sim n^{2 \nu}$.
$R$ behaves as $n$ in $1 \mathrm{~d}, n^{3 / 4}$ in $2 \mathrm{~d}, n^{0.59}$ in $3 \mathrm{~d}, \sim n^{1 / 2}(\ln n)^{1 / 8}$ and $n^{1 / 2}$ for $d>d_{c}=4$. Flory's formula is known as $\nu=\frac{3}{d+2}$.

## Flory's formula



$$
\begin{aligned}
& \vec{r}=\vec{a}_{1}+\vec{a}_{2}+\cdots+\vec{a}_{N} \\
& \left\langle\vec{r}^{2}\right\rangle \equiv\left\langle\sum_{i, j} \vec{a}_{i} \cdot \vec{a}_{j}\right\rangle=N a^{2} \\
& \left(\left\langle\vec{r}^{2}\right\rangle \equiv r^{2} \text { and } N a^{2} \equiv R_{0}^{2}\right) \\
& p_{d}(r) \sim \frac{1}{N^{3 / 2}} e^{-\frac{3}{2} \frac{r^{2}}{N a^{2}}}
\end{aligned}
$$

Free energy:

$$
F_{\text {elastic }}=E-T S=F(0)+\frac{3}{2} \frac{T r^{2}}{R_{0}^{2}}
$$

- Let $R$ is the linear size of a polymer chain of $N$ monomers.
$-c_{\text {int }}=\frac{N}{R^{d}}$ is the density of monomers.
$-f_{\text {rep }}=\frac{1}{2} T v(T) c^{2}$ is the repulsive energy per volume among monomers ( $c$ is local density of monomers); $\left\langle c^{2}\right\rangle \sim c_{\text {int }}^{2}$
- Free energy by repulsion is $F_{r e p} \sim T v(T) c^{2} R^{d} \sim T v \frac{N^{2}}{R^{d}}$
- Total free energy divided by $T: v \frac{N^{2}}{R^{d}}+\frac{3}{2} \frac{R^{2}}{R_{0}^{2}}$
$-R_{F}^{d+2} \sim v a^{2} N^{3} \rightarrow R_{f} \sim N^{3 /(d+2)} \rightarrow \nu=3 /(d+2)$.


## Self-avoiding loop

$P_{o}(n)$ is the probability to reach a neighbor of the starting position after $n$ steps. $P_{o}(n)=2 \sum_{\langle i, j\rangle} \Gamma_{i, j}(n) / \sum_{i, j} \Gamma_{i, j}(n)$.
$L(n)$ is the number of self-avoiding loops comprised of $n$ bonds.
$\frac{1}{N} \sum_{<i, j>} \Gamma_{i, j}(n)=(n+1) L(n+1)$
If $L(n)$ is scaled as $\sim n^{\alpha-3} \mu^{n}$, then $L(s)=\sum_{n=0}^{\infty} L(n) s^{n} \sim(1-\mu s)^{2-\alpha}$.
$P_{o}(n) \sim \frac{1}{n^{1-\alpha+\gamma}}$.


## $n$-vector cubic model

$$
-\beta H=K_{1} \sum_{<i, j>} s_{i} \cdot s_{j}+K_{2} \sum_{<i, j>}\left(s_{i} \cdot s_{j}\right)^{2}
$$

$s_{i} \cdot s_{j}=n \delta\left(\alpha_{i}, \alpha_{j}\right) \sigma_{i} \sigma_{j}$
$n$ is the dimension; $\alpha_{i}$ is the direction of spin $i\left(\alpha_{i}=1, \cdots, n\right)$; and $\sigma_{i}= \pm 1$ is an Ising spin at site $i$.
The partition function is

$$
\begin{aligned}
& Z=\underbrace{\frac{1}{(2 \pi)^{N}} \sum_{\left\{s_{i}\right\}} \prod_{<i j>} \underbrace{\exp \left[K_{1} \sum_{<i, j>} s_{i} \cdot s_{j}+K_{2} \sum_{<i, j>}\left(s_{i} \cdot s_{j}\right)^{2}\right]}_{1+\sinh n K_{1} e^{n^{2} K_{2}} \delta\left(\alpha_{i}, \alpha_{j}\right) \sigma_{i} \sigma_{j}+\left(e^{n^{2} K_{2}} \cosh n K_{1}-1\right) \delta\left(\alpha_{i}, \alpha_{j}\right)} . \underbrace{\operatorname{enc}}}_{\equiv \operatorname{Tr}} \\
& =\operatorname{Tr} \prod_{<i j>}\left[1+\tanh n K_{1} \delta\left(\alpha_{i}, \alpha_{j}\right) \sigma_{i} \sigma_{j}\right] \\
& =\operatorname{Tr} \prod_{<i j>}\left[1+v n \delta\left(\alpha_{i}, \alpha_{j}\right) \sigma_{i} \sigma_{j}\right] \quad \text { as } \quad n \rightarrow 0 \\
& =\operatorname{Tr} \prod_{<i j>}\left[1+v O_{i j}\right]=\sum_{G} v^{L} n^{C-N+L} \quad v \text { means a bond }
\end{aligned}
$$

$$
\begin{aligned}
Z= & \operatorname{Tr}\left(1+v O_{12}\right)\left(1+v O_{23}\right)\left(1+v O_{31}\right) \\
= & \operatorname{Tr}\left(1+3 v O_{12}+3 v^{2} O_{12} O_{23}+v^{3} O_{12} O_{23} O_{31}\right) \\
= & \sum_{\alpha_{1}=1}^{n} \sum_{\alpha_{2}=1}^{n} \sum_{\alpha_{3}=1}^{n} \sum_{\sigma_{1}=-1}^{\sigma_{1}=1} \sum_{\sigma_{2}=-1}^{\sigma_{2}=1} \sum_{\sigma_{3}=-1}^{\sigma_{3}=1} \\
& \left(1+3 v O_{12}+3 v^{2} O_{12} O_{23}+v^{3} O_{12} O_{23} O_{31}\right)
\end{aligned}
$$



## n-vector cubic model

where $G$ is graph, $C$ is the number of clusters, $L$ is the number of bonds, $S \equiv C-N+L$ is the cyclomatic number.
$L(\ell)$ is the number of loops of length $\ell$

$$
\begin{aligned}
Z & =1+n \sum_{\ell=0}^{\infty} N L(\ell) v^{\ell}+O\left(n^{2}\right) \\
-f & =\lim _{N \rightarrow \infty} \frac{1}{n N} \ln Z=\underbrace{\sum_{\ell=0}^{\infty} L(\ell) v^{\ell}}_{\text {the generating function of SA loop }}+O(n)
\end{aligned}
$$

P5') Consider a Sierpinski gasket. i) Obtain the fractal dimension. Consider random walks on an infinite Sierpinski gasket. ii) Obtain the spectral dimension and self-avoiding walk dimension $\nu$.
Note: P5 과 P5' 중 하나 선택

## Other random walks

i) Levy flight random walks (J-H Jeon)
ii) RWs with waiting times
iii) RWs in a random potential: Sinai's diffusion (J-H Jeon)
iv) RWs on complex networks (D.S. Lee)
vi) RWs on simplicial complexes. (Later)

## Contents

## (1) Overview

(2) References
(3) Diffusion, Random Walks on fractal structure

- Random walks
- Gaussian model
- Self-avoiding walks and $n$-vector cubic model
(4) Kinectics of reaction process
- Single-species annihilation/coalescence
- Two-species annihilation
- Two-species annihilation on fractal structure
- Two species annihilation on SF networks
(5) Aggregation


## Kinetics of reaction process

Single-species annihilation/coalescence
Two types of reactions:
i) Annihilation reaction: $A+A \xrightarrow{K} \phi$
ii) Coalescence reaction: $A+A \xrightarrow{K} A$
$\rho(t)$ is the density of $A$ particles.
Assume that the reactants are perfectly mixed at all times and thus the density at every site is always the same.
i) $\frac{d \rho}{d t}=-2 K \rho^{2} \Rightarrow \rho(t)=$

The true asymptotic behavior by the simulation that particles diffuse in the system and disappear when they meet.

$$
\text { But, } \quad \rho(t) \sim \begin{cases}, & d=1 \\ , & d=2 \\ , & d>2\end{cases}
$$

So there exists a critical dimension $d_{c}=2$. So there exists something more,

## Heuristic arguments

For the reaction $A+A \rightarrow \phi$, in a time interval $t$, each particle explores the region $\ell \sim \sqrt{D t}$ in $1 d$. the typical separation between surviving particles is of the order of $\ell$. $\Rightarrow \rho(t) \sim \ell^{-1} \sim(D t)^{-1 / 2}$.
More generally, the number of distinct sites $\mathcal{N}$ visited by a random walk after $n$ steps

$$
\mathcal{N} \sim \begin{cases}n^{1 / 2}, & d=1 \\ n / \ln n, & d=2 \\ n, & d>2\end{cases}
$$

Thus, it seems that $\rho(t) \sim n^{-1}$.

Two-species annihilation

electron-hole recombination, etc
$A+B \rightarrow \phi$ (when the densities of two species of particles are even)

$$
\rho(t) \sim \begin{cases} & d \leq 4 \\ t^{-1}, & d>4\end{cases}
$$

So the critical dimension is $d_{c}=4$. There is no logarithmic correction for $d=d_{c}$.
Heuristic argument
In a spatial region of linear size $\ell$, the initial number of $A$ particles is

$$
N_{A}=\rho_{0} \ell^{d} \pm \sqrt{\rho_{0} \ell^{d}} \quad \text { and } \quad N_{B}=\rho_{0} \ell^{d} \pm \sqrt{\rho_{0} \ell^{d}}
$$

$N_{A}-N_{B}= \pm \sqrt{\rho_{0} \ell^{d}}$. One of the species with population $\sqrt{\rho_{0} \ell^{d}}$ survive within the region of linear size $\ell$. Thus the local density becomes $\rho \sim \sqrt{\rho_{0} \ell^{d}} / \ell^{d}$. Because, $\ell \sim \sqrt{D t}$,

$$
\rho(t) \sim \sqrt{\rho_{0}}(D t)^{-d / 4} \quad \text { and } \quad \frac{d \rho}{d t} \sim D \sqrt{\rho_{0}}(D t)^{-d / 4-1}
$$

## Three scales


i) the average distance between neighboring particles $\ell_{A A} \sim \rho^{-1 / d} \sim \rho_{0}^{-1 / 2} t^{d / 4}$.
ii) Domain linear size: $t$ 시간 동안 입자들은 $L$ 만큼 영역 내에서 random walks 를 하므로 그 영역 내에서 $A+B \rightarrow 0$ 의 reaction 이 일어 날 것이고 그 중 majority 가 살아 남아 domain 을 만들 것이다. 그러므로 domain size 는 $L \sim \sqrt{D t}$ 이 됨.
iii) The distance between two particles of different species, $\ell_{A B}$.

1-i) For 1 d , a typical AB pair reacts in a time $\Delta t \sim \ell_{A B}^{2} / D$.
1-ii) The number of reactions per unit length per domain:
$\Delta \rho \sim O(1 / L) \sim O(1 / \sqrt{D t})$, where $L$ is domain size.
1-iii) $\Delta \rho / \Delta t \sim-(D t)^{-1 / 2} /\left(\ell_{A B}^{2} / D\right)$.
1 -iv) Thus, $\ell_{A B} \sim[\rho(0)]^{-1 / 4}(D t)^{3 / 8}$.

2-i) For 2d, a typical AB pair reacts in a time $\Delta t \sim \ell_{A B}^{2} / D$.
2-ii) The number of reactions per unit length per domain: $\Delta \rho$ is of the order of $\left[(D t)^{1 / 2} / \ell_{A B}\right] /(\sqrt{D t})^{2}$, where $L$ is domain size.
2-iii) $\Delta \rho / \Delta t \sim \frac{\left[(D t)^{1 / 2} / \ell_{A B}\right] /(\sqrt{D t})^{2}}{\ell_{A B}^{2} / D}$.
2-iv) Thus, $\ell_{A B} \sim[\rho(0)]^{-1 / 6}(D t)^{1 / 3}$.
For $d=3$, random walks are transient, so $\ell_{A B}=\ell_{A A} \sim t^{1 / 4}$.

Two-species annihilation on fractal structure

## Heuristic argument

$$
\begin{aligned}
& A+B \rightarrow \phi \\
& \rho(t) \sim \begin{cases}t^{-d_{s} / 4}, & d_{s} \leq 4 \\
t^{-1}, & d_{s}>4\end{cases}
\end{aligned}
$$

So the critical dimension is $d_{s, c}=4$.
There is no logarithmic correction for $d_{s}=d_{c}$.

In a spatial region of linear size $\ell$, the initial number of $A$ particles is

$$
N_{A}=\rho_{0} \ell^{d_{f}} \pm \sqrt{\rho_{0} \ell^{d_{f}}} \quad \text { and } \quad N_{B}=\rho_{0} \ell^{d_{f}} \pm \sqrt{\rho_{0} \ell^{d_{f}}}
$$

$N_{A}-N_{B}= \pm \sqrt{\rho_{0} \ell^{d_{f}}}$. One of the species with population $\sqrt{\rho_{0} \ell^{d_{f}}}$ survive within the region of linear size $\ell$. Thus the local density becomes $\rho \sim \sqrt{\rho_{0} \ell^{d_{f}}} / \ell^{d_{f}}$. Because, $\ell \sim(D t)^{1 / d_{w}}$,

$$
\rho(t) \sim \sqrt{\rho_{0}}(D t)^{-d_{s} / 4} \quad \text { and } \quad \frac{d \rho}{d t} \sim D \sqrt{\rho_{0}}(D t)^{-d_{s} / 4-1}
$$

Three scales on fractal structure


Challenging project 1)
Determine $\ell_{A A}, \ell_{A B}$, and Domain size $L$ in terms of $d_{f}$ and $d_{S}$.

## Two species annihilation on SF networks

$A+B \rightarrow 0$ on fractal SF networks (Yun, et al., NJP (2009))
A fractal SF network is constructed: At each branching step, a node creates its $m$ branches with probability $p_{m} \sim m^{-\gamma}$ with $\langle m\rangle=1$.

$$
\begin{gathered}
d_{f}=\left\{\begin{array}{ll}
\frac{\gamma-1}{\gamma-2}, & \text { for } 2<\gamma<3, \\
2, & \text { for } \gamma>3
\end{array} \quad d_{s}= \begin{cases}\frac{2(\gamma-1)}{2 \gamma-3}, & \text { for } 2<\gamma<3, \\
\frac{4}{3}, & \text { for } \gamma>3\end{cases} \right. \\
d_{w}=\frac{2 d_{f}}{d_{s}}
\end{gathered}
$$

i) $\frac{1}{\rho(t)}-\frac{1}{\rho(t)} \sim t^{d_{s} / 4}$
ii) The linear size of a domain $L \sim t^{1 / d_{w}}$.
iii) $\ell_{A A} \sim \rho(t)^{-1 / d_{f}} \sim t^{1 /\left(2 d_{w}\right)}$.
iv) $N_{A A} \sim\left(1 / \ell_{A A}^{d_{f}}\right) \rho(t) \sim t^{-d_{s} / 2}$ and $N_{A B} \propto d \rho / d t \sim t^{-d_{s} / 4-1}$

## Other reactions

i) For $A_{1}+A_{2}+\cdots+A_{N} \rightarrow \phi$, when the densities of each species are even, $\rightarrow \rho(t) \sim t^{-d / 4}$ independent of $N$ for $d<d_{c}=4 /(N-1)$, but for $d>d_{c}, \rho(t) \sim t^{-1 /(N-1)}$
ii) For $N A \rightarrow \phi$, under the same condition of i), $\rho(t) \sim t^{-d / 2}$ for $d<d_{c}=2 /(N-1)$, but $\rho(t) \sim t^{-1 /(N-1)}$ for $d>d_{c}$
iii) $A_{i}+A_{j} \xrightarrow{K_{i j}} A_{i \pm 1}+A_{j \mp 1}$ solvable.

P6) Show i) and ii)

## Contents

(1) Overview

- References
(3) Diffusion, Random Walks on fractal structure
- Random walks
- Gaussian model
- Self-avoiding walks and $n$-vector cubic model
(9) Kinectics of reaction process
- Single-species annihilation/coalescence
- Two-species annihilation
- Two-species annihilation on fractal structure
- Two species annihilation on SF networks
(5) Aggregation


## Aggregation <br> An example

## Diffusion limited cluster aggregation



Order parameter
$m(t)=\frac{S_{g}(t)}{N}$
Mean cluster size
$\langle s\rangle$
Correlation length
$\xi$

Aggregation of grease spots in a frypan

## Aggregation

An example


## Aggregation

Blood coagulation, milk curdling, star formation, etc.

$$
A_{i}+A_{j} \xrightarrow{K_{i j}} A_{i+j}
$$

The master equation (Smoluchowski equation for $K_{i j}=1$ ) under the conditions: Spatial homogeneity, Bimolecular reactions (ignoring higher-body interactions), and then shape independence. $c_{k}(t)=N_{k}(t) / N$

$$
\frac{d c_{k}}{d t}=\frac{1}{2} \sum_{i+j=k} K_{i j} c_{i} c_{j}-c_{k} \sum K_{i k} c_{i}
$$

$\Rightarrow M_{1}(t) \equiv \sum_{k=1} k c_{k}(t)=1$ is conserved. That is, $\frac{d M_{1}}{d t}=0$

## i) Kernel of Brownian motion

$K_{i j} \sim\left(D_{i}+D_{j}\right)\left(R_{i}+R_{j}\right):$
$D_{i}$ is diffusion constant $D_{i} \propto 1 / R_{i}$ (Stoke-Einstein relation), where $R_{i}$ is radius of a cluster of size $i$. Clusters are regarded as spheres. So contact is made in 1 d way. $R_{i} \sim i^{1 / 3}$ in 3 d .
$K_{i j} \sim\left(i^{-1 / 3}+j^{-1 / 3}\right)\left(i^{1 / 3}+j^{1 / 3}\right) \sim 2+\left(\frac{i}{j}\right)^{1 / 3}+\left(\frac{j}{i}\right)^{1 / 3}$
This kernel is not constant. But it satisfies the scaling behavior $K_{i, j}=K_{a i, a j}$. Thus, $K_{i j}=2$ is considered.

$$
\dot{c}_{k}=\sum_{i+j=k} c_{i} c_{j}-2 c_{k} \underbrace{\sum_{i=1} c_{i}}_{M_{0}(t)}
$$

with an initial condition $c_{k}(0)=\delta_{k, 1}$.
i) Kernel of Brownian motion $K_{i j}=2$

Moments

Define the moment of the mass distribution $M_{n}(t) \equiv \sum_{k=1} k^{n} c_{k}(t)$.

$$
\begin{array}{lr}
\dot{M}_{n}=\sum_{i, j}(i+j)^{n} c_{i} c_{j}-2 M_{n} M_{0} & \\
\dot{M}_{0}=-M_{0}^{2} & M_{0}=1 /(1+t) \\
\dot{M}_{1}=0 & M_{1}=1 \\
\dot{M}_{2}=2 M_{1}^{2} & M_{2}=1+2 t \\
\dot{M}_{3}=6 M_{1} M_{2} & M_{3}=1+6 t+6 t^{2} \\
& M_{n} \simeq n!t^{n-1}
\end{array}
$$

i) Kernel of Brownian motion $K_{i j}=2$
cluster size distribution: Exponential ansatz

Suppose $c_{k}(t)=A(t) a(t)^{k-1}$

$$
\dot{c}_{k}=\sum_{i+j=k} c_{i} c_{j}-2 c_{k}
$$

This equation must be held for any $k$. So $\dot{A}=-\frac{2 A^{2}}{1-a}, \dot{a}=A$.
We use $\sum_{k} k c_{k}=1$ to get $A=(1-a)^{2}$. Then $a=\frac{t}{1+t}$ and $A=\frac{1}{(1+t)^{2}}$
$\rightarrow c_{k}(t)=\frac{t^{k-1}}{(1+t)^{k+1}}$
i) Kernel of Brownian motion $\quad K_{i j}=2$

Generating function method
$g(z, t)=\sum_{k=1} c_{k}(t) z^{k}$

$$
\begin{aligned}
\frac{d g}{d t} & =\sum_{k=1} \sum_{i+j=k} c_{i} z^{i} c_{j} z^{j}-2 \sum_{k=1} c_{k} z^{k} \sum_{i} c_{i}=g^{2}-2 g M_{0} \\
& =g^{2}-2 g M_{0}+M_{0}^{2}-M_{0}^{2} \\
\frac{d\left(g-M_{0}\right)}{d t} & =g^{2}-2 g M_{0}+M_{0}^{2}=\left(g-M_{0}\right)^{2} \\
g & =\frac{1}{1+t} \frac{z}{1-(z-1) t}=\sum_{k} z^{k} \frac{t^{k-1}}{(1+t)^{k+1}} \\
c_{k}(t) & =\frac{t^{k-1}}{(1+t)^{k+1}}
\end{aligned}
$$

P7) Suppose that the cluster size dist. at $t=0$ is given by $c_{k}(0)=b k^{-\gamma}$, where $2<\gamma<3$. Solve the generating function $g(z, t)$ and $c_{k}(t)$.
ii) Gelation $K_{i j}=i j$


A monomer has three branches (reactive endgroups). Then two monomers are merged and produce a dimer with four branches. When one monomer and one dimer are merged, a trimer has five branches. Generally, $k$-mer has $(f-2) k+2$ branches, where $f$ is the number of branches of a monomer.
$K_{i j}=[(f-2) i+2][(f-2) j+2]=(f-2)^{2} i j+2(f-2)(i+j)+4$

$$
\dot{c}_{k}=\frac{1}{2} \sum_{i+j=k} i j c_{i} c_{j}-k c_{k} \overbrace{\sum_{i=1}^{=1} i c_{i}}^{=1}
$$

Moments : Gelation (giant cluster of infinite size)
Sol-Gel transition. Suppose a system of $N$ monomers. As time passes, two clusters are merged and generate a bigger cluster. This process is repeated. At a certain time step, a cluster of size $m N$ of $O(1)$ emerges, called a Gel.
"Mass" means size of a cluster. Consider the moments of the mass distribution $c_{k}$. For $t<1$,

$$
\begin{aligned}
\frac{d M_{2}}{d t} & =\sum_{k=1} k^{2} \frac{d c_{k}}{d t}=\frac{1}{2} \sum_{i=1} \sum_{j=1}(i+j)^{2}\left(i c_{i}\right)\left(j c_{j}\right)-\sum_{k=1} k^{3} c_{k} \\
& =\sum_{i} \sum_{j}\left(i^{2} c_{i}\right)\left(j^{2} c_{j}\right)=M_{2}^{2} \quad \rightarrow \quad M_{2}(t)=\frac{M_{2}(0)}{1-M_{2}(0) t} \\
\frac{d M_{3}}{d t} & =3 M_{3} M_{2} \quad \rightarrow \quad M_{3}(t)=\frac{M_{3}(0)}{\left(1-M_{2}(0) t\right)^{3}} \\
\frac{d M_{4}}{d t} & =4 M_{4} M_{2}+3 M_{3}^{2}
\end{aligned}
$$

## Moments for $t>1$

$$
\begin{aligned}
& M_{n}(t)=\sum_{k} k^{n} c_{k}=\sum_{\text {sol }} k^{n} c_{k}+\left(k^{n} c_{k}\right)_{\mathrm{gel}} \\
& M_{0}(t)=\sum_{\text {sol }} c_{k} \\
& M_{1}(t)=\sum_{\text {sol }} k c_{k}+m \\
& M_{2}(t)=\sum_{\text {sol }} k^{2} c_{k}+m^{2} N \\
& M_{3}(t)=\sum_{\text {sol }} k c_{k}+m^{3} N^{2}
\end{aligned}
$$

## Generating function approach

$$
\begin{aligned}
& g(y, t) \equiv \sum_{k} k c_{k}(t) e^{y k} \\
& \begin{aligned}
& \frac{\partial g(y, t)}{\partial t}=\frac{1}{2} \sum_{i=1} \sum_{j=1}(i+j) i j c_{i} c_{j} e^{y k}-\sum_{k=1} k^{2} c_{k} e^{y k} \\
&=\frac{1}{2} \sum_{i=1} i^{2} c_{i} e^{y i} \sum_{j=1} j c_{j} e^{y j}+\frac{1}{2} \sum_{i=1} i c_{i} e^{y i} \sum_{j=1} j^{2} c_{j} e^{y j} \\
&-\sum_{k=1} k^{2} c_{k} e^{y k} \\
&=(g-1) \frac{\partial g}{\partial y} \\
& \frac{\frac{d g}{d t}=\frac{\partial g}{\partial t}+(1-\mathcal{E}) \frac{\partial g}{\partial y}=0}{\frac{d g}{d t}=\frac{\partial g}{\partial t}+\frac{d y}{d t} \frac{\partial g}{\partial y}=0}
\end{aligned}
\end{aligned}
$$

To solve this first-order PDE, one may need to find a quantity along which $g(y, t)$ remains constant. $d g / d t=0$.
As usual, we take $\frac{d y}{d t}=1-g$ as an invariant quantity over time.
$y=(1-g) t+f(g) . f(g)$ is determined from the initial condition.
$g=\sum_{k} k c_{k}(t) e^{y k} \xrightarrow{t=0} e^{y}$.
So $y=(1-g) t+\ln g \rightarrow g e^{-g t}=e^{y-t}$
Set $Y=g t$ and $X=t e^{y-t}$ and then $X=Y e^{-Y}$
Given a function $X=f(Y)$ with $X \simeq Y$ for small $Y$, What is $Y(X)=\sum_{n=1} A_{n} X^{n}$ ?
Using Lagrange inversion formula $A_{N}=\frac{n^{n-1}}{n!}$

$$
g(y, t)=\sum_{k} \frac{k^{k-1}}{k!} t^{k-1} e^{-k t} e^{y k} \Rightarrow c_{k}(t)=\frac{k^{k-2}}{k!} t^{k-1} e^{-k t}
$$

$c_{k}(t)=\frac{k^{k-2}}{k!} t^{k-1} e^{-k t} \xrightarrow{t \rightarrow 1^{-}} \frac{e^{-k(1-t)^{2} / 2}}{\sqrt{2 \pi} k^{5 / 2}} \simeq s^{-5 / 2} \Phi(k / s)$ for $t \leq 1$ with $\Phi(x)=\frac{1}{\sqrt{2 \pi}} \frac{e^{-x / 2}}{x^{5 / 2}}$ and $s=(1-t)^{-2}$.

The stirling's formula: $n!\sim \sqrt{2 \pi n}\left(\frac{n}{e}\right)^{n}$
For $t>1$, the fraction of nodes in the giant cluster:
$m=1-M_{1}=1-g(y=0, t) \equiv 1-g_{0}(t)$.
Using the relation $g_{0}=e^{-\left(1-g_{0}\right) t}, 1-m=e^{-m t}$.
To solve $g$ near $t=1^{+}$, let $t=1+\delta . \Rightarrow m=2 \delta=2(t-1)+\cdots$.

$$
m(t)=1-\sum_{k} k c_{k}(t)=\frac{2 M_{2}^{2}(0)}{M_{3}(0)}\left(M_{2}(0) t-1\right)
$$

## $M_{2}(t)$ for $t>t_{c}$

$$
\begin{aligned}
& \frac{d M_{2}(t)}{d t}=\frac{1}{2} \sum_{i} \sum_{j}(i+j)^{2} i j c_{i} c_{j}-\sum_{k} k^{3} c_{k} \\
& =\sum_{i} \sum_{j} i^{2} c_{i} j^{2} c_{j}+\sum_{i} i^{3} c_{i} \underbrace{\sum_{j} j c_{j}}_{\neq 1}-\sum_{k} k^{3} c_{k} \\
& =M_{2}^{2}-m M_{3} \\
& M_{n}=\left.\frac{\partial^{n-1} g}{\partial y^{n-1}}\right|_{y=0} \\
& M_{2}(t)=\sum_{k} k^{2} c_{k}(t)= \begin{cases}(1-t)^{-1}, & \text { for } t<1, \\
\left(e^{m t}-t\right)^{-1}, & \text { for } t>1 .\end{cases}
\end{aligned}
$$



## Lagrange inversion formula:

Given a function $X=f(Y)$ with $X \simeq Y$ for small $Y$,
What is $Y(X)=\sum_{n=1} A_{n} X^{n}$ ?

$$
\begin{aligned}
A_{n} & =\frac{1}{2 \pi i} \oint \frac{Y}{X^{n+1}} d X=\frac{1}{2 \pi i} \oint \frac{Y}{X^{n+1}} \frac{d X}{d Y} d Y \\
& =\frac{1}{2 \pi i} \oint \frac{Y}{f(Y)^{n+1}} f^{\prime}(x) d Y \\
& =\frac{1}{2 \pi i} \oint \frac{Y}{\left(Y e^{-Y}\right)^{n+1}}(1-Y) e^{-Y} d Y=\frac{1}{2 \pi i} \oint \frac{1-Y}{Y^{n}} e^{n Y} d Y \\
& =\frac{1}{2 \pi i} \oint \sum_{k=0} \frac{n^{k}}{k!}\left(Y^{k-n}-Y^{k+1-n}\right) d Y=\frac{n^{n-1}}{n!}
\end{aligned}
$$

## Loops (cycles)

E. Ben-Naim and P.L. Krapivsky, PRE 71, 026129 (2005)

Model ER model

- $\exists N$ nodes. Links are generated with rate $1 /(2 N)$
- self-loop and multiple links are allowed
- the average number of links: $L=\frac{N^{2} t}{2 N}=\frac{N t}{2}$
- the average number of self-loops $C=\frac{N t}{2 N}=\frac{t}{2}$
- mean degree $t$, transition point $t_{c}=1$
- cluster size dist at $t_{c}: c_{k} \sim k^{-5 / 2}(\tau=5 / 2)$
- $N \sum_{k=k_{m}}^{\infty} c_{k} \sim 1 \rightarrow k_{m} \sim N^{2 / 3}$ (Giant cluster size).

Tree

- $q_{\ell}(t)$ is the density of distinct paths of length $\ell$ at time $t$

$$
\frac{d q_{\ell}}{d t}=\sum_{n+m=\ell-1} q_{n} q_{m}, \quad \text { with } \quad q_{0}(t)=1
$$

- $q_{\ell}(0)=\delta_{\ell, 0}$, then $q_{0}(t)=1, q_{1}(t)=t, q_{2}(t)=t^{2}, \ldots q_{\ell}(t)=t^{\ell}$


## Path length

## Path length density in finite systems

- $p_{\ell, k}$ is the density of distinct paths of length $\ell$ in components of size $k$

$$
\frac{d p_{\ell, k}}{d t}=\sum_{\substack{i+j=k, n+m=\ell-1}} p_{n, i} p_{m, j}+\sum_{i+j=k} i p_{\ell, i} j c_{j}-k p_{\ell, k}
$$

- $p_{\ell, k}=(\ell+1) \frac{k^{k-\ell-2}}{(k-\ell-1)!} t^{k-1} e^{-k t}$ for $t<t_{c}=1$
- the characteristic length $\ell_{c} \sim(1-t)^{-1} \rightarrow \sigma_{\ell}=1$
- $p_{\ell, k}=\ell\left(2 \pi k^{3}\right)^{-1 / 2} \exp \left(-\ell^{2} / 2 k\right)$ at $t=t_{c} . \ell \sim \sqrt{k} \sim N^{1 / 3}$

Cycles

- $w_{\ell}$ is the density of cicles of size $\ell$ at time $t$.
- $\frac{d w_{\ell}}{d t}=\frac{N q_{\ell-1}}{2 N}=\frac{t^{\ell-1}}{2}, \rightarrow w_{\ell}=\frac{t^{\ell}}{2 \ell} \rightarrow w_{\ell}=\frac{1}{2 \ell}$ at $t_{c}=1$.

Cycles in finite systems

- $u_{\ell, k}(t)$ is the average number of unicyclic of length $\ell$ contained in the components of size $k$ at time $t$.

$$
\frac{d u_{\ell, k}}{d t}=\frac{1}{2} p_{\ell-1, k}+\sum_{i+j=k} i u_{\ell, i} j c_{j}-k u_{\ell, k} \quad \text { with } \quad u_{\ell, k}(0)=0
$$

- $u_{\ell, k}(t) \simeq\left(8 \pi k^{3}\right)^{-1 / 2} t^{k} e^{k(1-t)} e^{-\ell^{2} / 2 k}$
- $u_{\ell, k}(t) \simeq \ell^{-3} \Phi_{u}\left(k(1-t)^{2}, \ell(1-t)\right)$ near $t \rightarrow t_{c}^{-}$
- $\gamma=1$


## Other Kernels

i) when $K_{i j} \sim i+j: c_{k}\left(t_{c}\right) \sim k^{-2}$ but as $t_{c} \rightarrow \infty$.
ii) when $K_{i j} \sim(i j)^{\omega}: c_{k}\left(t_{c}\right) \sim k^{-\tau}$ with

$$
\tau=\left\{\begin{array}{lll}
\frac{3}{2}+\omega, & \text { for } \frac{1}{2}<\omega<1 & \text { at finite } t_{c} \\
1+2 \omega, & \text { for } 0<\omega<\frac{1}{2} & \text { at infinite } t_{c}
\end{array}\right.
$$

Refs: Ziff, et al., PRL 49, 593 (1982).
Cho et al., PRE 81, 030103(R) (2010).

## Scaling theory

The scaling ansatz: Assume $c(s, t)=\frac{1}{s^{* 2}} f\left(\frac{s}{s^{*}}\right)$.
Because, $\int s c(s, t) d x=1$ is required. $M_{n}=\int s^{n} \frac{1}{s^{* 2}} f\left(\frac{s}{s^{*}}\right) d x \sim s^{*(n-1)}$
Assume that $K(a i, a j) \sim a^{\lambda} K(i, j)$,

$$
\frac{\partial c}{\partial t}=\frac{1}{2} \int_{0}^{x} d y K(y, x-y) c(y, t) c(x-y, t)-\int_{0}^{\infty} d y K(x, y) c(x, t) c(y, t)
$$

Plugging $c(s, t)=s^{*-2} f\left(s / s^{*}\right)$ into the Smol. Eq.
LHS $\rightarrow \frac{\partial c}{\partial t}=-\frac{\dot{s}^{*}}{s^{* 3}}\left[2 f(u)+u f^{\prime}(u)\right] u=x / s^{*}$.
RHS $\rightarrow s^{*(\lambda-3)} \mathcal{K}(u)$ (with $\left.v=y / s\right)$

$$
\mathcal{K}(u)=\frac{1}{2} \int_{0}^{u} d v K(v, u-v) f(v) f(u-v)-\int_{0}^{\infty} d v K(u, v) f(u) f(v)
$$

$$
\begin{gathered}
\frac{\dot{s}^{*}(t)}{s^{* \lambda}(t)}=-\frac{\mathcal{K}(u)}{2 f(u)+u f^{\prime}(u)} \equiv \Lambda \\
s^{*}(t) \sim \begin{cases}t^{1 /(1-\lambda)} \equiv t^{z}, & \text { for } \lambda<1 \\
e^{\Lambda t}, & \text { for } \lambda=1 \\
\left(t_{g}-t\right)^{-1 /(\lambda-1)}, & \text { for } 1<\lambda \leq 2\end{cases}
\end{gathered}
$$

$2 f(u)+u f^{\prime}(u)+\Lambda^{-1} \mathcal{K}(u)=0 \Leftarrow$ the way to solve it is not developed yet.

## Aggregation with input

## constant kernel

At $t=0, c_{k}(0)=0$. At each time step, a monomer is added to the system.

$$
\begin{aligned}
& \frac{d c_{k}}{d t}=\sum_{i+j=k} c_{i} c_{j}-2 c_{k} \underbrace{\sum_{i} c_{i}}_{M_{0}}+\delta_{k, 1} \\
& M_{0}(t)=\tanh t .
\end{aligned}
$$

$\dot{M}_{0}=-M_{0}^{2}+1 \rightarrow M_{0}(t)=\tanh t$.
g-function $\mathcal{C}(z, t)=\sum_{k} c_{k}(t) z^{k}$.

$$
\frac{d \mathcal{C}(z, t)}{d t}=\mathcal{C}^{2}-2 \mathcal{C} M_{0}+z \rightarrow \frac{d \mathcal{C}-M_{0}}{d t}=\left(\mathcal{C}-M_{0}\right)^{2}+(z-1)
$$

$\mathcal{C}(z, t)=\tanh t-\sqrt{1-z} \tanh (t \sqrt{1-z})$.
As $t \rightarrow \infty, \mathcal{C}(z, t)=1-\sqrt{1-z} . \rightarrow c_{k} \simeq \frac{1}{\sqrt{4 \pi}} \frac{1}{k^{3 / 2}}$
Because $\sum k c_{k}(t)=1, \exists$ a cutoff $k^{*}$ s.t. $\sum_{k=1}^{k^{*}} k c_{k}(t)=1$. So $k^{*} \sim t^{2}$.
For $k>k^{*}, c_{k}(t)=\frac{\pi^{2}}{4 t^{3}} e^{-\pi^{2} k / 4 t^{2}}$.

## Aggregation with spatially localized input

$$
\frac{d c_{k}}{d t}=D \nabla^{2} c_{k}+\sum_{i+j=k} c_{i} c_{j}-2 c_{k} \sum_{i} c_{i}+J \delta_{k, 1} \delta(x)
$$

At $t=0, c_{k}(0)=0$. At each time step, a monomer is added to the system. $M_{1}=\sum_{k} k c_{k}$

$$
\frac{\partial M_{1}}{\partial t}=D \nabla^{2} M_{1}+J \delta(x)
$$

P8)

$$
M_{1}(t) \xrightarrow{t \rightarrow \infty} \begin{cases}? & \text { for } d=1 \\ ? & \text { for } d=2 \\ ? & \text { for } d=3\end{cases}
$$

Aggregation in Euclidean space Research papers by Meakin and Family Y.S.Cho and B.Kahng," Discontinuous percolations in real physical systems," Phys.Rev. E 84, 050102(R) (2011).

