Kinetic models in statistical physics

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- Random walks
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- Two-species annihilation
- Two-species annihilation on fractal structure
- Two species annihilation on SF networks

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Aggregation

Where are we now?

Q1 통계물리학에서는 어떤 주제를 연구했었는가?

Q2 최근에는 어떤 주제를 연구하는가?

Q3 어떤 중요한 연구 문제가 남아있는가?

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Random walks

(I) $P_n(x)$ is the occupation probability at site x at time step n.

$$P_n(x) = pP_{n-1}(x-1) + qP_{n-1}(x+1)$$

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. $\prod_n(r) = \binom{n}{r}p^rq^{n-r}.$ Using the stirling's approximation and x = 2r - n, $\boxed{n! \sim \sqrt{2\pi n}(\frac{n}{e})^n}$

$$P_n(x) = \prod_n [(x+n)/2] = \frac{1}{\sqrt{2\pi n p q}} e^{-[x-n(p-q)]^2/2npq}$$

= $\frac{1}{\sqrt{2\pi n \sigma^2}} e^{-[x-n\langle x \rangle]^2/2n\sigma^2}$
= $\frac{1}{\sqrt{4\pi D n}} e^{-[x-n\langle x \rangle]^2/4Dn} \quad \langle x^2 \rangle = 2Dt$

Random walks (II) The master equation:

(*n* is a position)

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

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

$$\boxed{e^{x\cos k} = \sum_{n=-\infty}^{\infty} e^{ikn}I_n(x)} \rightarrow P_n(t) = I_n(2t)e^{-2t} \xrightarrow{t \to \infty} \frac{1}{\sqrt{4\pi t}}e^{-n^2/4t}$$

Modified Bessel function:

$$I_n(x) = \frac{1}{2\pi i} \oint e^{(x/2)(t+1/t)} t^{-n-1} dt$$

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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.

$$P_{i,j}(n) = \sum_{j_1} W_{j_1,j} P_{i,j_1}(n-1) = \sum_{j_1} W_{j_1,j} \sum_{j_2} W_{j_2,j_1} P_{i,j_2}(n-2)$$
$$= \dots = \sum_{j_1} \sum_{j_2} \dots \sum_{l} W_{j_1,j} W_{j_2,j_1} \dots W_{j_{n-1} \to j_{n-2}} W_{i,j_{n-1}}$$
$$= (W^n)_{i,j}$$

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

$$\mathcal{P}_{i,j}(s) \equiv \sum_{n=0}^{\infty} P_{i,j}(n) s^n = \sum_{n=0}^{\infty} (W^n)_{i,j} s^n = \left(\frac{1}{I - sW}\right)_{i,j}$$
$$= \left(\frac{1}{(1 - s)I + swV}\right)_{i,j}$$

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In Euclidean lattice

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

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

 z_i : coordination number of site i s.t. $1 - z_i w \ge 0$

Laplacian matrix
$$V_{i,j} \equiv \begin{cases} -1 & (i,j) \text{ is n.n} \\ z_i & i = j \\ 0 & \text{otherwise} \end{cases}$$

$$\Rightarrow W = I - wV$$

Generally,

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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 $P_o(n)$:

$$\mathcal{P}_o(s) \equiv \sum_{n=0}^{\infty} P_o(n) s^n = \frac{1}{N} \sum_i \left(\frac{1}{(1-s)I + swV} \right)_{i,i}$$
$$= \frac{1}{N} \sum_{\ell} \frac{1}{(1-s) + sw\lambda_{\ell}}$$
$$= \int_0^{\infty} \frac{\rho_s(\lambda) d\lambda}{1 - s(1-w\lambda)} = \sum_{n=0} \int_0^{\infty} s^n (1-w\lambda)^n \rho_s(\lambda) d\lambda$$

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Image: A matrix and a matrix

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$$\Rightarrow P_o(n) = \int_0^\infty (1 - w\lambda)^n \rho_s(\lambda) d\lambda \approx \int_0^\infty e^{-nw\lambda} \rho_s(\lambda) d\lambda,$$

where $\rho_s(\lambda)$ is the spectral density of Laplacian matrix V.

P1) Show the following:

Consider a harmonic motion: $m \frac{d^2 x_i}{dt^2} = -k \sum_{j \in n.n. \text{ of } i} (x_i - x_j)$ $\lambda x_i = \sum_j V_{i,j} x_j$ Then the eigenvalue $\lambda \sim \omega^2$, and the spectral density is $\rho_s(\lambda) \sim \lambda^{\frac{d_s}{2}-1}$

 $(d_s: \text{ spectral dimension})$

P2) Show the following: $\Rightarrow P_o(n) \sim n^{-d_s/2} \Rightarrow \mathcal{P}_o(s) \sim (1-s)^{\frac{d_s}{2}-1} \rightarrow \text{singular when } d_s < 2 \text{ as}$ $s \rightarrow 1.$

Mean distance

 R_{ij} is the distance from site *i* to *j* Mean distance after *n* time steps: (d_w : random-walk dimension)

$$\langle R_n^2 \rangle = \frac{1}{N} \sum_i \sum_j R_{ij}^2 P_{i,j}(n) \sim n^{2/d_w}$$

 $R^2(s) = \sum_{n=0}^{\infty} \langle R_n^2 \rangle s^n \sim \sum_n n^{2/d_w} s^n \sim$

 $\langle R_n^2\rangle=2Dn$ 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: $P_o(n) \sim \frac{1}{M} \sim n^{-d_f/d_w} \sim n^{-d_s/2}$

$$d_w = \frac{2d_f}{d_s}$$

 \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:

$$f(s) = \int_0^\infty t^{-\mu} e^{-st} dt$$

= $s^{\mu-1} \int_0^\infty x^{-\mu} e^{-x} dx = \Gamma(1-\mu) s^{\mu-1}$

$$\Gamma(z) = \int_0^\infty x^{z-1} e^{-x} dx$$

$$\begin{split} R^2(s) &\sim \sum_n n^{2/d_w} s^n \sim \sum_n n^{2/d_w} e^{n \ln s} \quad \text{for} \quad 0 < s < 1 \\ &\sim \sum_n n^{2/d_w} e^{-n(1-s)} \sim \Gamma(2/d_w + 1)(1-s)^{-(2/d_w + 1)} \end{split}$$

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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.

$$P(r,t) = \int_0^t F(r,t') P(0,t-t') dt' + \delta_{r,0} \delta(0)$$

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: $\mathcal{R} = F_L(0,0) = \int_0^\infty F(0,t)dt$ 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 $t \to \infty$,

P3) Show that $F(t) \simeq \frac{1}{\sqrt{\pi}} \frac{1}{t^{3/2}}$ in 1d; $F(t) \simeq \frac{4\pi}{t(\ln t)^2}$ in 2d; and $F(t) \simeq \frac{(1-\mathcal{R})^2}{8\pi^{3/2}} \frac{1}{t^{3/2}}$ in 3d. Find \mathcal{R} in 3d.

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 $x_2>x_1.$

$$c(y,t) = \frac{1}{\sqrt{8\pi Dt}} \left[e^{-(y-y_0)^2/8Dt} - e^{-(y+y_0)^2/8Dt} \right]$$

P4) show that $F(t) \sim \frac{y_0}{\sqrt{8\pi Dt^3}} e^{-y_0^2/8Dt} \sim t^{-3/2}$ The survival probability $S(t) = 1 - \frac{2}{\sqrt{\pi}} \int_{y_0/\sqrt{8Dt}}^{\infty} e^{-u^2} du \rightarrow \frac{y_0}{\sqrt{2\pi Dt}}$ Gaussian model: a spin model of RWs

$$-\beta H = \beta \sum_{\langle i,j \rangle} W_{i,j} \phi_i \phi_j + \sum_i h_i \phi_i,$$

 ϕ_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

$$Z = \int [d\phi] e^{-\sum_{i} \phi_{i}^{2} + \beta \sum_{\langle ij \rangle} W_{ij} \phi_{i} \phi_{j} + \sum_{i} h_{i} \phi_{i}}$$
$$= \prod_{l} \left[\frac{\pi}{1 - \beta \lambda_{l}} \right]^{\frac{1}{2}} \exp\left[(\sum_{i} h_{i} a_{il})^{2} / 4(1 - \beta \lambda_{l}) \right]$$

Internal energy: With $h_i = 0$,

$$u = -\frac{1}{N} \frac{\partial}{\partial \beta} (\ln Z) = \underline{\qquad}$$
$$= \frac{1}{2\beta} \left(1 - \frac{1}{N} \sum_{i} \frac{1}{I - \beta W} \right)_{ii}$$

because $\sum_{j} W_{i,j} = 1$, $a_{i,0} = \frac{1}{\sqrt{N}}$ and $\lambda_0 = 1$. $\sum_{l} a_{il}a_{jl} = \delta_{i,j}$

$$u \sim \left(1 - \frac{\beta}{\beta_c}\right)^{1 - \alpha_g} \Leftrightarrow \mathcal{P}_o(s) \sim (1 - s)^{\frac{d_s}{2} - 1}$$
$$1 - \alpha_g = \frac{d_s}{2} - 1 \Rightarrow 2 - \alpha_g = \frac{d_s}{2} = \frac{d_f}{d_w} = d_f \nu_g$$

Correlation function

$$\Gamma_{ij} = \frac{\partial^2 \ln Z}{\partial h_i \partial h_j} = \langle \phi_i \phi_j \rangle - \langle \phi_i \rangle \langle \phi_j \rangle$$
$$= \frac{1}{2} \sum_l \frac{a_{il} a_{jl}}{1 - \beta \lambda_l} = \frac{1}{2} \left(\frac{1}{I - \beta W} \right)_{i,j} \Leftrightarrow \mathcal{P}_{i \to j}(\beta)$$

Susceptibility

$$\chi = \frac{1}{N} \sum_{i,j} \Gamma_{i,j} = \frac{1}{2N} \sum_{i,j,l} \frac{a_{il}a_{jl}}{1 - \beta\lambda_l} = \underline{\qquad},$$

because $\sum_{j} W_{i,j} = 1$, $a_{i,0} = \frac{1}{\sqrt{N}}$ and $\lambda_0 = 1$. $\sum_{l} a_{il}a_{jl} = \delta_{i,j}$ $\gamma_g = 1$

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Correlation length

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

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

$$R^{2}(s) = \xi^{2}(s)\chi(s) \sim (1-s)^{-2\nu_{g}-\gamma_{g}} \sim (1-s)^{-2\nu_{g}-1}$$
$$R^{2}_{n} \sim n^{2\nu_{g}} \qquad (\nu_{g} = 1/d_{w})$$

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





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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: $N_i(n) = \sum_j \Gamma_{i,j}(n)$

$$\begin{split} N(n) &= \frac{1}{N} \sum_{i} N_{i}(n) \text{ and } N(s) = \sum_{n} N(n) s^{n}. \\ \text{If } N(n) &\sim n^{\gamma - 1} \mu^{n}, \text{ then } N(s) \sim (1 - \mu s)^{-\gamma}, \text{ where } \mu = 1/s_{c}. \\ \langle R^{2}(n) \rangle &= \sum_{i,j} R_{ij}^{2} \Gamma_{ij} / \sum_{i,j} \Gamma_{ij} \sim n^{2\nu}. \end{split}$$

R behaves as n in 1d, $n^{3/4}$ in 2d, $n^{0.59}$ in 3d, $\sim n^{1/2}(\ln n)^{1/8}$ and $n^{1/2}$ for $d>d_c=4.$ Flory's formula is known as $\nu=\frac{3}{d+2}.$

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Flory's formula



- Let R is the linear size of a polymer chain of N monomers.
- $-c_{int} = \frac{N}{R^d}$ is the density of monomers.
- $f_{rep} = \frac{1}{2}Tv(T)c^2$ is the repulsive energy per volume among monomers (c is local density of monomers); $\langle c^2 \rangle \sim c_{int}^2$
- Free energy by repulsion is $F_{rep} \sim Tv(T)c^2R^d \sim Tv \frac{N^2}{R^d}$
- Total free energy divided by $T: v \frac{N^2}{R^4} + \frac{3}{2} \frac{R^2}{R^2}$
- $R_F^{d+2} \sim va^2 N^3 \to R_f \sim N^{3/(d+2)} \to \nu = 3/(d+2).$

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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 $L(s) = \sum_{n=0}^{\infty} L(n)s^n \sim (1-\mu s)^{2-\alpha}$.





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n-vector cubic model

$$-\beta H = K_1 \sum_{\langle i,j \rangle} s_i \cdot s_j + K_2 \sum_{\langle i,j \rangle} (s_i \cdot s_j)^2$$

 $s_i \cdot s_j = n\delta(\alpha_i, \alpha_j)\sigma_i\sigma_j$ n is the dimension; α_i is the direction of spin i ($\alpha_i = 1, \dots, n$); and $\sigma_i = \pm 1$ is an Ising spin at site i.

The partition function is

$$Z = \underbrace{\frac{1}{(2\pi)^N} \sum_{\{s_i\}} \prod_{\langle ij \rangle}}_{\equiv \operatorname{Tr}} \underbrace{\exp\left[K_1 \sum_{\langle i,j \rangle} s_i \cdot s_j + K_2 \sum_{\langle i,j \rangle} (s_i \cdot s_j)^2\right]}_{1+\sinh nK_1 e^{n^2 K_2} \delta(\alpha_i, \alpha_j) \sigma_i \sigma_j + (e^{n^2 K_2} \cosh nK_1 - 1) \delta(\alpha_i, \alpha_j)}$$

$$= \operatorname{Tr} \prod_{\langle ij \rangle} [1 + \tanh nK_1 \delta(\alpha_i, \alpha_j) \sigma_i \sigma_j]$$

$$= \operatorname{Tr} \prod_{\langle ij \rangle} [1 + vn\delta(\alpha_i, \alpha_j) \sigma_i \sigma_j] \quad \text{as} \quad n \to 0$$

$$= \operatorname{Tr} \prod_{\langle ij \rangle} [1 + vO_{ij}] = \sum_{G} v^L n^{C-N+L} \quad v \text{ means a bond}$$

$$= \operatorname{Tr} \prod_{\langle ij \rangle} [1 + vO_{ij}] = \sum_{G} v^L n^{C-N+L} \quad v \text{ means a bond}$$

$$= \operatorname{Tr} \prod_{\langle ij \rangle} [1 + vO_{ij}] = \sum_{G} v^L n^{C-N+L} \quad v \text{ means a bond}$$

$$Z = Tr(1 + vO_{12})(1 + vO_{23})(1 + vO_{31})$$

= $Tr(1 + 3vO_{12} + 3v^2O_{12}O_{23} + v^3O_{12}O_{23}O_{31})$
= $\sum_{\alpha_1=1}^n \sum_{\alpha_2=1}^n \sum_{\alpha_3=1}^n \sum_{\sigma_1=-1}^{\sigma_1=1} \sum_{\sigma_2=-1}^{\sigma_2=1} \sum_{\sigma_3=-1}^{\sigma_3=-1} (1 + 3vO_{12} + 3v^2O_{12}O_{23} + v^3O_{12}O_{23}O_{31})$

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Kinetic models

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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 ℓ

$$\begin{split} Z &= 1 + n \sum_{\ell=0}^{\infty} NL(\ell) v^{\ell} + O(n^2) \\ -f &= \lim_{N \to \infty} \frac{1}{nN} \ln Z = \sum_{\substack{\ell=0 \\ \ell = 0}}^{\infty} L(\ell) v^{\ell} + O(n) \\ & \text{the generating function of SA loop} \end{split}$$

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 ν . Note: P5 과 P5' 중 하나 선택

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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)

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- Two-species annihilation on fractal structure
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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.

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Assume that the reactants are perfectly mixed at all times and thus the density at every site is always the same.

i)
$$\frac{d\rho}{dt} = -2K\rho^2 \quad \Rightarrow \quad \rho(t) =$$

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

$$\label{eq:But} {\rm But}, \quad \rho(t) \sim \left\{ \begin{array}{ccc} & , & d=1\,, \\ & , & d=2\,, \\ & , & d>2\,. \end{array} \right.$$

So there exists a critical dimension $d_c = 2$. So there exists something more,

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Heuristic arguments

For the reaction $A + A \rightarrow \phi$,

in a time interval t, each particle explores the region $\ell \sim \sqrt{Dt}$ in 1d. the typical separation between surviving particles is of the order of ℓ . $\Rightarrow \rho(t) \sim \ell^{-1} \sim (Dt)^{-1/2}$.

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 $A+B \rightarrow \phi \text{ (when the densities of two species of particles are even)}$

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

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 ℓ , the initial number of A particles is

$$N_A = \rho_0 \ell^d \pm \sqrt{\rho_0 \ell^d}$$
 and $N_B = \rho_0 \ell^d \pm \sqrt{\rho_0 \ell^d}$

 $N_A - N_B = \pm \sqrt{\rho_0 \ell^d}$. One of the species with population $\sqrt{\rho_0 \ell^d}$ survive within the region of linear size ℓ . Thus the local density becomes $\rho \sim \sqrt{\rho_0 \ell^d} / \ell^d$. Because, $\ell \sim \sqrt{Dt}$,

$$\rho(t) \sim \sqrt{\rho_0} (Dt)^{-d/4} \quad \text{and} \quad \frac{d\rho}{dt} \sim D\sqrt{\rho_0} (Dt)^{-d/4-1}$$

Three scales

i) the average distance between neighboring particles $\ell_{AA} \sim \rho^{-1/d} \sim \rho_0^{-1/2} t^{d/4}$.

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 $L \sim \sqrt{Dt}$ 이 됨.

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iii) The distance between two particles of different species, ℓ_{AB} .

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

2-iii) $\Delta \rho / \Delta t \sim \frac{[(Dt)^{1/2}/\ell_{AB}]/(\sqrt{Dt})^2}{\ell_{AB}^2/D}$.

2-iv) Thus, $\ell_{AB} \sim [\rho(0)]^{-1/6} (Dt)^{1/3}$.

For d=3, random walks are transient, so $\ell_{AB}=\ell_{AA}\sim t^{1/4}$.

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Two-species annihilation on fractal structure



$$A + B \rightarrow \phi$$

$$\rho(t) \sim \begin{cases} t^{-d_s/4}, & d_s \le 4, \\ t^{-1}, & d_s > 4. \end{cases}$$

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

Heuristic argument

In a spatial region of linear size ℓ , the initial number of A particles is

$$N_A = \rho_0 \ell^{d_f} \pm \sqrt{\rho_0 \ell^{d_f}}$$
 and $N_B = \rho_0 \ell^{d_f} \pm \sqrt{\rho_0 \ell^{d_f}}$

 $N_A - N_B = \pm \sqrt{\rho_0 \ell^{d_f}}$. One of the species with population $\sqrt{\rho_0 \ell^{d_f}}$ survive within the region of linear size ℓ . Thus the local density becomes $\rho \sim \sqrt{\rho_0 \ell^{d_f}} / \ell^{d_f}$. Because, $\ell \sim (Dt)^{1/d_w}$,

$$\rho(t) \sim \sqrt{\rho_0} (Dt)^{-d_s/4} \quad \text{and} \quad \frac{d\rho}{dt} \sim D\sqrt{\rho_0} (Dt)^{-d_s/4-1}$$

Three scales on fractal structure



Challenging project 1) Determine ℓ_{AA} , ℓ_{AB} , and Domain size L in terms of d_f and d_s .

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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 $\langle m \rangle = 1$.

$$\begin{split} d_f &= \begin{cases} \frac{\gamma - 1}{\gamma - 2}, & \text{for} \quad 2 < \gamma < 3, \\ 2, & \text{for} \quad \gamma > 3. \end{cases} \qquad d_s = \begin{cases} \frac{2(\gamma - 1)}{2\gamma - 3}, & \text{for} \quad 2 < \gamma < 3, \\ \frac{4}{3}, & \text{for} \quad \gamma > 3. \end{cases} \\ \end{split}$$

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 $NA \rightarrow \phi$, 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) $A_i + A_j \xrightarrow{K_{ij}} A_{i\pm 1} + A_{j\mp 1}$ solvable.

P 6) Show i) and ii)

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Aggregation

Aggregation

An example

Diffusion limited cluster aggregation



Aggregation

An example



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Aggregation

Blood coagulation, milk curdling, star formation, etc.

$$A_i + A_j \xrightarrow{K_{ij}} A_{i+j}$$

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

$$\frac{dc_k}{dt} = \frac{1}{2} \sum_{i+j=k} K_{ij} c_i c_j - c_k \sum K_{ik} c_i$$

 $\Rightarrow M_1(t) \equiv \sum_{k=1} k c_k(t) = 1$ is conserved. That is, $\frac{dM_1}{dt} = 0$

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i) Kernel of Brownian motion

$$K_{ij} \sim (D_i + D_j)(R_i + R_j):$$

 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 1d way. $R_i \sim i^{1/3}$ in 3d.

$$K_{ij} \sim (i^{-1/3} + j^{-1/3})(i^{1/3} + j^{1/3}) \sim 2 + \left(\frac{i}{j}\right)^{1/3} + \left(\frac{j}{i}\right)^{1/3}$$

This kernel is not constant. But it satisfies the scaling behavior $K_{i,j} = K_{ai,aj}$. Thus, $K_{ij} = 2$ is considered.

$$\dot{c}_k = \sum_{i+j=k} c_i c_j - 2c_k \sum_{\substack{i=1\\M_0(t)}} c_i$$

with an initial condition $c_k(0) = \delta_{k,1}$.

i) Kernel of Brownian motion $K_{ij} = 2$ Moments

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

$$\begin{split} \dot{M}_n &= \sum_{i,j} (i+j)^n c_i c_j - 2M_n M_0 \\ \dot{M}_0 &= -M_0^2 & M_0 = 1/(1+t) \\ \dot{M}_1 &= 0 & M_1 = 1 \\ \dot{M}_2 &= 2M_1^2 & M_2 = 1+2t \\ \dot{M}_3 &= 6M_1 M_2 & M_3 = 1+6t+6t^2 \\ & M_n \simeq n! t^{n-1} \end{split}$$

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i) Kernel of Brownian motion $K_{ij} = 2$

cluster size distribution: Exponential ansatz

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

$$\dot{c}_k = \sum_{i+j=k} c_i c_j - 2c_k$$

This equation must be held for any k. So $\dot{A} = -\frac{2A^2}{1-a}$, $\dot{a} = A$. We use $\sum_k kc_k = 1$ 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

$$K_{ij} = 2$$

Generating function method

 $g(z,t) = \sum_{k=1} c_k(t) z^k$

$$\begin{aligned} \frac{dg}{dt} &= \sum_{k=1}^{N} \sum_{i+j=k}^{N} c_i z^i c_j z^j - 2 \sum_{k=1}^{N} c_k z^k \sum_i c_i = g^2 - 2gM_0 \\ &= g^2 - 2gM_0 + M_0^2 - M_0^2 \\ \frac{d(g - M_0)}{dt} &= g^2 - 2gM_0 + M_0^2 = (g - M_0)^2 \\ g &= \frac{1}{1+t} \frac{z}{1-(z-1)t} = \sum_k z^k \frac{t^{k-1}}{(1+t)^{k+1}} \\ c_k(t) &= \frac{t^{k-1}}{(1+t)^{k+1}} \end{aligned}$$

P7) Suppose that the cluster size dist. at t = 0 is given by $c_k(0) = bk^{-\gamma}$, where $2 < \gamma < 3$. Solve the generating function g(z, t) and $c_k(t)$.

ii) Gelation $K_{ij} = ij$



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.

$$K_{ij} = [(f-2)i+2][(f-2)j+2] = (f-2)^2ij + 2(f-2)(i+j) + 4$$

$$\dot{c}_k = \frac{1}{2} \sum_{i+j=k} i j c_i c_j - k c_k \sum_{i=1}^{j=1} i c_i$$

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 mN 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,

$$\begin{aligned} \frac{dM_2}{dt} &= \sum_{k=1} k^2 \frac{dc_k}{dt} = \frac{1}{2} \sum_{i=1} \sum_{j=1} (i+j)^2 (ic_i) (jc_j) - \sum_{k=1} k^3 c_k \\ &= \sum_i \sum_j (i^2 c_i) (j^2 c_j) = M_2^2 \quad \rightarrow \quad M_2(t) = \frac{M_2(0)}{1 - M_2(0)t} \\ \frac{dM_3}{dt} &= 3M_3 M_2 \quad \rightarrow \quad M_3(t) = \frac{M_3(0)}{(1 - M_2(0)t)^3} \\ \frac{dM_4}{dt} &= 4M_4 M_2 + 3M_3^2 \end{aligned}$$

Moments for t > 1

$$M_n(t) = \sum_k k^n c_k = \sum_{\text{sol}} k^n c_k + (k^n c_k)_{\text{gel}}$$
$$M_0(t) = \sum_{\text{sol}} c_k$$
$$M_1(t) = \sum_{\text{sol}} k c_k + m$$
$$M_2(t) = \sum_{\text{sol}} k^2 c_k + m^2 N$$
$$M_3(t) = \sum_{\text{sol}} k c_k + m^3 N^2$$

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Generating function approach

$$\begin{split} g(y,t) &\equiv \sum_{k} kc_{k}(t)e^{yk} \\ &\frac{\partial g(y,t)}{\partial t} = \frac{1}{2} \sum_{i=1} \sum_{j=1} (i+j)ijc_{i}c_{j}e^{yk} - \sum_{k=1} k^{2}c_{k}e^{yk} \\ &= \frac{1}{2} \sum_{i=1} i^{2}c_{i}e^{yi} \sum_{j=1} jc_{j}e^{yj} + \frac{1}{2} \sum_{i=1} ic_{i}e^{yi} \sum_{j=1} j^{2}c_{j}e^{yj} \\ &- \sum_{k=1} k^{2}c_{k}e^{yk} \\ &= (g-1)\frac{\partial g}{\partial y} \\ \hline \frac{dg}{dt} &= \frac{\partial g}{\partial t} + (1-\mathcal{E})\frac{\partial g}{\partial y} = 0 \\ \hline \frac{dg}{dt} &= \frac{\partial g}{\partial t} + \frac{dy}{dt}\frac{\partial g}{\partial y} = 0 \end{split}$$

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To solve this first-order PDE, one may need to find a quantity along which g(y,t) remains constant. dg/dt = 0.

As usual, we take $\frac{dy}{dt} = 1 - g$ as an invariant quantity over time. y = (1 - g)t + f(g). f(g) is determined from the initial condition. $g = \sum_{k} kc_k(t) e^{yk} \xrightarrow{t=0} e^y.$ So $y = (1 - q)t + \ln q \to q e^{-gt} = e^{y-t}$ Set Y = qt and $X = te^{y-t}$ and then $X = Ye^{-Y}$ Given a function X = f(Y) with $X \simeq Y$ for small Y. What is $Y(X) = \sum_{n=1}^{\infty} A_n X^n?$ Using Lagrange inversion formula $\left|A_N = \frac{n^{n-1}}{n!}\right|$

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

$$\begin{split} c_k(t) &= \frac{k^{k-2}}{k!} t^{k-1} e^{-kt} \xrightarrow{t \to 1^-} \frac{e^{-k(1-t)^2/2}}{\sqrt{2\pi}k^{5/2}} \simeq s^{-5/2} \Phi(k/s) \text{ for } t \leq 1 \\ \text{with } \Phi(x) &= \frac{1}{\sqrt{2\pi}} \frac{e^{-x/2}}{x^{5/2}} \text{ and } s = (1-t)^{-2}. \end{split}$$

The stirling's formula: $\boxed{n! \sim \sqrt{2\pi n} (\frac{n}{e})^n}$

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 $g_0 = e^{-(1-g_0)t}$, $1 - m = e^{-mt}$.

To solve g near $t = 1^+$, let $t = 1 + \delta$. $\Rightarrow m = 2\delta = 2(t - 1) + \cdots$.

$$m(t) = 1 - \sum_{k} kc_k(t) = \frac{2M_2^2(0)}{M_3(0)}(M_2(0)t - 1)$$

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 $M_2(t)$ for $t > t_c$

$$\frac{dM_2(t)}{dt} = \frac{1}{2} \sum_i \sum_j (i+j)^2 i j c_i c_j - \sum_k k^3 c_k$$
$$= \sum_i \sum_j i^2 c_i j^2 c_j + \sum_i i^3 c_i \sum_{\substack{j \\ \neq 1}} j c_j - \sum_k k^3 c_k$$

$$= M_2^2 - mM_3$$

$$M_n = \frac{\partial^{n-1}g}{\partial y^{n-1}}\Big|_{y=0}$$

$$M_2(t) = \sum_k k^2 c_k(t) = \begin{cases} (1-t)^{-1}, & \text{ for } t < 1, \\ (e^{mt} - t)^{-1}, & \text{ for } t > 1. \end{cases}$$

Kahng (SNU)

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Lagrange inversion formula:

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

$$A_{n} = \frac{1}{2\pi i} \oint \frac{Y}{X^{n+1}} dX = \frac{1}{2\pi i} \oint \frac{Y}{X^{n+1}} \frac{dX}{dY} dY$$

$$= \frac{1}{2\pi i} \oint \frac{Y}{f(Y)^{n+1}} f'(x) dY$$

$$= \frac{1}{2\pi i} \oint \frac{Y}{(Ye^{-Y})^{n+1}} (1-Y) e^{-Y} dY = \frac{1}{2\pi i} \oint \frac{1-Y}{Y^{n}} e^{nY} dY$$

$$= \frac{1}{2\pi i} \oint \sum_{k=0} \frac{n^{k}}{k!} (Y^{k-n} - Y^{k+1-n}) dY = \frac{n^{n-1}}{n!}$$

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Loops (cycles)

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

- $\exists \ N$ nodes. Links are generated with rate 1/(2N)
- self-loop and multiple links are allowed
- the average number of links: $L = \frac{N^2 t}{2N} = \frac{N t}{2}$
- the average number of self-loops $C = \frac{Nt}{2N} = \frac{t}{2}$
- mean degree t, transition point $t_c = 1$
- cluster size dist at t_c : $c_k \sim k^{-5/2}$ (au = 5/2)

•
$$N \sum_{k=k_m}^{\infty} c_k \sim 1 \rightarrow k_m \sim N^{2/3}$$
 (Giant cluster size).
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• $q_\ell(t)$ is the density of distinct paths of length ℓ at time t

$$\frac{dq_\ell}{dt} = \sum_{n+m=\ell-1} q_n q_m, \quad \text{with} \quad q_0(t) = 1$$

• $q_{\ell}(0) = \delta_{\ell,0}$, then $q_0(t) = 1$, $q_1(t) = t$, $q_2(t) = t^2$, ... $\left| q_{\ell}(t) = t^{\ell} \right|$

Path length

Path length density in finite systems

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

$$\frac{dp_{\ell,k}}{dt} = \sum_{\substack{i+j=k, \\ n+m=\ell-1}} p_{n,i}p_{m,j} + \sum_{i+j=k} ip_{\ell,i}jc_j - kp_{\ell,k}$$

•
$$p_{\ell,k} = (\ell+1) \frac{k^{k-\ell-2}}{(k-\ell-1)!} t^{k-1} e^{-kt}$$
 for $t < t_c = 1$

• the characteristic length $\ell_c \sim (1-t)^{-1} \rightarrow \sigma_\ell = 1$

•
$$p_{\ell,k} = \ell (2\pi k^3)^{-1/2} \exp(-\ell^2/2k)$$
 at $t = t_c$. $\ell \sim \sqrt{k} \sim N^{1/3}$

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Cycles

• w_{ℓ} is the density of cicles of size ℓ at time t.

•
$$\frac{dw_\ell}{dt} = \frac{Nq_{\ell-1}}{2N} = \frac{t^{\ell-1}}{2}$$
, $\rightarrow w_\ell = \frac{t^\ell}{2\ell} \rightarrow w_\ell = \frac{1}{2\ell}$ at $t_c = 1$.

Cycles in finite systems

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

$$\frac{du_{\ell,k}}{dt} = \frac{1}{2}p_{\ell-1,k} + \sum_{i+j=k} iu_{\ell,i}jc_j - ku_{\ell,k} \quad \text{with} \quad u_{\ell,k}(0) = 0$$

•
$$u_{\ell,k}(t) \simeq (8\pi k^3)^{-1/2} t^k e^{k(1-t)} e^{-\ell^2/2k}$$

• $u_{\ell,k}(t) \simeq \ell^{-3} \Phi_u(k(1-t)^2, \ell(1-t))$ near $t \to t_c^-$
• $\gamma = 1$

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Other Kernels

i) when
$$K_{ij} \sim i + j$$
: $c_k(t_c) \sim k^{-2}$ but as $t_c \to \infty$.

ii) when $K_{ij} \sim (ij)^{\omega}$: $c_k(t_c) \sim k^{-\tau}$ with

$$\tau = \begin{cases} \frac{3}{2} + \omega, & \text{ for } \frac{1}{2} < \omega < 1 & \text{ at finite } t_c, \\ 1 + 2\omega, & \text{ for } 0 < \omega < \frac{1}{2} & \text{ at infinite } t_c. \end{cases}$$

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

Image: A matrix and a matrix

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Scaling theory

The scaling ansatz: Assume $c(s,t) = \frac{1}{s^{*2}}f(\frac{s}{s^*})$. Because, $\int sc(s,t)dx = 1$ is required. $M_n = \int s^n \frac{1}{s^{*2}}f(\frac{s}{s^*})dx \sim s^{*(n-1)}$

Assume that $K(ai, aj) \sim a^{\lambda} K(i, j)$,

$$\frac{\partial c}{\partial t} = \frac{1}{2} \int_0^x dy K(y, x - y) c(y, t) c(x - y, t) - \int_0^\infty dy K(x, y) c(x, t) c(y, t)$$

Plugging $c(s,t) = s^{*-2}f(s/s^*)$ into the Smol. Eq. LHS $\rightarrow \frac{\partial c}{\partial t} = -\frac{\dot{s}^*}{s^{*3}}[2f(u) + uf'(u)] \ u = x/s^*.$ RHS $\rightarrow s^{*(\lambda-3)}\mathcal{K}(u)$ (with v = y/s)

$$\mathcal{K}(u) = \frac{1}{2} \int_0^u dv K(v, u - v) f(v) f(u - v) - \int_0^\infty dv K(u, v) f(u) f(v)$$

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$$\begin{split} \frac{\dot{s}^*(t)}{s^{*\lambda}(t)} &= -\frac{\mathcal{K}(u)}{2f(u) + uf'(u)} \equiv \Lambda\\ s^*(t) \sim \begin{cases} t^{1/(1-\lambda)} \equiv t^z, & \text{for } \lambda < 1,\\ e^{\Lambda t}, & \text{for } \lambda = 1\\ (t_g - t)^{-1/(\lambda - 1)}, & \text{for } 1 < \lambda \leq 2. \end{cases} \end{split}$$

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

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Aggregation with input constant kernel

At t = 0, $c_k(0) = 0$. At each time step, a monomer is added to the system.

$$\begin{aligned} \frac{dc_k}{dt} &= \sum_{i+j=k} c_i c_j - 2c_k \sum_{i} c_i + \delta_{k,1} \\ \dot{M}_0 &= -M_0^2 + 1 \to M_0(t) = \tanh t. \end{aligned}$$
g-function $\mathcal{C}(z,t) &= \sum_k c_k(t) z^k.$

$$\frac{d\mathcal{C}(z,t)}{dt} &= \mathcal{C}^2 - 2\mathcal{C}M_0 + z \to \frac{d\mathcal{C} - M_0}{dt} = (\mathcal{C} - M_0)^2 + (z-1) \\ \mathcal{C}(z,t) &= \tanh t - \sqrt{1-z} \tanh(t\sqrt{1-z}). \end{aligned}$$
As $t \to \infty$, $\mathcal{C}(z,t) = 1 - \sqrt{1-z}. \to c_k \simeq \frac{1}{\sqrt{4\pi}} \frac{1}{k^{3/2}}$
Because $\sum_i kc_k(t) = 1$, \exists a cutoff k^* s.t. $\sum_{k=1}^{k^*} kc_k(t) = 1$. So $k^* \sim t^2$.
For $k > k^*$, $c_k(t) = \frac{\pi^2}{4t^3} e^{-\pi^2 k/4t^2}.$

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Aggregation with spatially localized input

$$\frac{dc_k}{dt} = D\nabla^2 c_k + \sum_{i+j=k} c_i c_j - 2c_k \sum_i c_i + J\delta_{k,1}\delta(x)$$

At $t=0,\,c_k(0)=0.$ At each time step, a monomer is added to the system. $M_1=\sum_k k c_k$

$$\frac{\partial M_1}{\partial t} = D\nabla^2 M_1 + J\delta(x)$$

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$$M_1(t) \xrightarrow{t \to \infty} \begin{cases} ? & \text{for } d = 1, \\ ? & \text{for } d = 2 \\ ? & \text{for } d = 3. \end{cases}$$

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).

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