Lecture Note on

"Fundamentals of Walk Models and First Passage Problem"

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Prologue

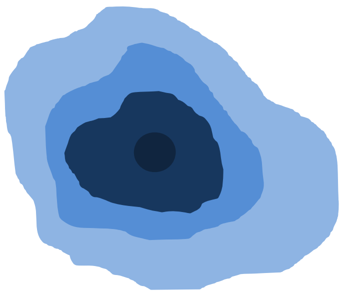
- **Meaning of random walks (RWs).**

  통계물리학자의 마음의 고향 (비빌 언덕).

  - Ising Model (70-80%).
  - Random walks (20-30%).

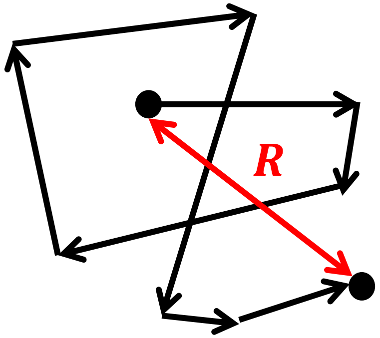
- **RWs : static (configurational) or dynamic model?**

  ① Diffusion – Dynamic phenomena.



$$\langle R^2 \rangle \sim t^{2\nu} \qquad (t = \text{time})$$

  ② Polymer structure : static configurational problem.



$$\langle R^2 \rangle \sim \langle R_g^2 \rangle \sim N^{2\nu} \qquad \begin{pmatrix} N : \text{monomer 수} \\ \text{step 수} \end{pmatrix}$$

- **Chapter 1. General properties of random walks.**

(Main Refs. [1], [2], [*])

§1. Markovian process.

§2. Central limit Theorem.

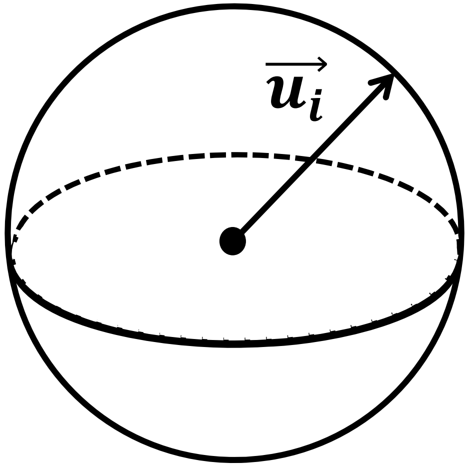
§3. Recursion Relation.

§4. Master Equation.

§5. Diffusion Equation.

§5. RWs on finite-sized system.

§1. Markovian process of first order : philosophy of $\left\{\begin{matrix}\text{pure}\\ \text{true}\end{matrix}\right\}$ random walks(RWs).



* $\overrightarrow{u_i}$: the hopping vector at the ith hopping (philosophy ①).

$$\left(\begin{matrix}\langle\overrightarrow{u_i}\rangle = 0\\ |\overrightarrow{u_i}| = u\\ \left\langle\overrightarrow{u_i^2}\right\rangle = u^2\end{matrix}\right) \quad \text{(philosophy ②)} \tag{1}$$

After N hoppings,

$$\vec{R}(N) = \sum_{i=1}^{N} \overrightarrow{u_i} \tag{2}$$

$$\langle\vec{R}(N)\rangle = \sum_{i=1}^{N} \langle\overrightarrow{u_i}\rangle = 0 \tag{3}$$

$$\langle\vec{R}^2(N)\rangle = \left\langle\left(\sum_{i=1}^{N}\overrightarrow{u_i}\right)\cdot\left(\sum_{j=1}^{N}\overrightarrow{u_j}\right)\right\rangle = \left\langle\sum_{i=1}^{N}\overrightarrow{u_i}^2\right\rangle + \left\langle\sum_{i=1}^{N}\sum_{(i\neq j)}^{N}\overrightarrow{u_i}\cdot\overrightarrow{u_j}\right\rangle \tag{4}$$

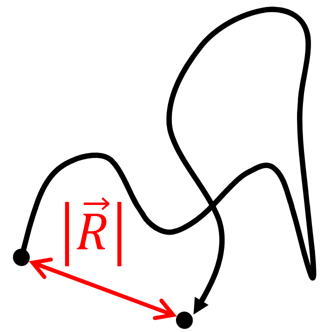
If $\langle \vec{u_i} \cdot \vec{u_j} \rangle = 0$ for $\forall$ $(i < j)$ with $i \neq j$, **(5)**
(no memory effect : philosophy ③ → Markovian process of first order).

$$\langle \vec{R}^2(N) \rangle = N u^2 \quad \left(\nu = \frac{1}{2}\right) \tag{6}$$

* Definition of Exponents

***1.** End-to-end distance exponent, ν.

$$R_E^2 \equiv \langle \vec{R}^2(N) \rangle \sim N^{2\nu} \tag{7}$$



***2.** No. of N-step possible walkers, γ.

$$\mathcal{J}_N \sim N^{\gamma - 1} \mu^N \tag{8}$$

$\mathcal{J}_N$ of RWs on hyper cubic lattices with coordination number z :

$$\mathcal{J}_N = z^N \quad (\gamma = 1, \mu = z) \tag{9}$$

from Markovian process (μ =effective coordination #).

(Excercise) Prove that $\langle \vec{R}^4 \rangle \sim 3N^2 u^4$ or $\langle \vec{R}^4 \rangle / 3 \langle \vec{R}^2 \rangle^2 = 1$
in the limit $N \to \infty$.

§2. Central limit theorem

*Philosophy 1 : The unit hopping time is finite const.

(→ violation → continuous time RWs)

*Philosophy 2 :

$$\int p(\overrightarrow{u_i}) d^d u_i = 1$$

$$\int \overrightarrow{u_i}\ p(\overrightarrow{u_i})\ d^d u_i = finite\ vector$$

$$\int \overrightarrow{u_i}^2\ p(\overrightarrow{u_i})\ \ d\overrightarrow{u_i} = finite\ number \qquad \textbf{(10)}$$

(→ violation → Lévy flight)

*Philosophy 3 : $\left\{ \begin{array}{l} \text{No memory Effect. (Markovian process of first order.)} \\ \text{No interaction between monomers in polymers.} \end{array} \right.$

(→ violation → $\left\{ \begin{array}{l} \text{Persistent RWs} \\ \text{Self-avoiding walks} \\ \text{Other walk models} \end{array} \right\}$)

* 문제를 간단히 하기 위해 1차원에서 생각해 보자
(강의의 모든 walk는 원점에서 출발한다고 가정함)

기본걸음의 PDF $p(u) \rightarrow \begin{cases} \langle u \rangle = \int p(u) u \, du = m_1 \\ \langle u^2 \rangle = \int p(u) u^2 \, du \ , \ \ m_2 = \langle u^2 \rangle - \langle u \rangle^2 \end{cases}$

N step 후 RW의 위치 $R(N)$: $R(N) = u_1 + u_2 + \cdots + u_N$

$$P(R,N) = \int_{-\infty}^{\infty} du_1 \, p(u_1) \ldots \int_{-\infty}^{\infty} du_N \, p(u_N) \ \delta\left(R - \sum_{i=1}^{N} u_i \right)$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \, e^{ikR} \prod_{i=1}^{N} \int_{-\infty}^{\infty} du_i e^{-iku_i} p(u_i)$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \, e^{ikR} \, [Q(k)]^N$$

$$Q(k) = \int du \, p(u) \ e^{-iku}$$

$$Q(k) = 1 - ik\langle u \rangle - k^2 \langle u^2 \rangle / 2 \qquad (k \rightarrow 0)$$

$$\approx e^{(-ikm_1 - k^2 m_2/2)} \qquad (\ m_1 = \langle u_1 \rangle, \ \ m_2 = \langle u^2 \rangle - \langle u \rangle^2, \ \ \ldots \ )$$

$$P(R,N) = \frac{1}{(2\pi\, m_2\, N)^{\frac{1}{2}}} \exp\left(-\frac{(R - Nm_1)^2}{2m_2 N}\right) \qquad \textbf{(11)}$$

($m_1 = \langle u_1 \rangle \neq 0$: Biased RW)

$$P(R,N) = N^{-\nu} f\left(\frac{R_s}{N^{\nu}}\right) \qquad \textbf{(12)}$$

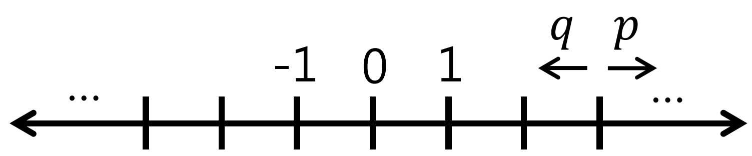
($R_s = R - Nm$, $\nu = 1/d_w = 1/2$), (d_w: RWs의 fractal dimension ($d_w = 2$))

Eq. (12)→ RW's Central limit theorem(CLT) → scaling property

§3. Recursion Relation

1d : Biased RW : $P(u) = p\delta(u-1) + q\delta(u+1)$

($p = q = \frac{1}{2}$, pure random walk)



Recursion Relation : $P(n,N) = pP(n-1,N-1) + qP(n+1,N)$ **(13)**

Generating function

$$\tilde{P}(n,K) = \sum_{N=0}^{\infty} P(n,N)K^N \qquad (K : \text{Fugacity}) \tag{14}$$

On 1d chain $\left(-\frac{L}{2}, \frac{L}{2}\right)$

$$f(k) = \sum_{n=-\frac{L}{2}}^{L/2} e^{ikn} f(n) \qquad \left(k = \frac{2\pi l}{L}\ ; l = -\frac{L}{2}, \ldots, \frac{L-1}{2}\right)$$

(Fourier transform : $L \to \infty$)

From Eq (13)

$$\tilde{P}(k,K) = \sum_{N=0}^{\infty} \sum_{n} e^{ikn} P(n,N) K^{N} \tag{15}$$

$$\tilde{P}(k,K) - 1 = K u(k) \tilde{P}(k,K)$$

$$\begin{cases} P(n,0) = \delta_{n0} \\ u(k) = p e^{ik} + q e^{-ik} \end{cases} \tag{16}$$

$$\tilde{P}(k,K) = \frac{1}{1 - K u(k)} = \sum_{N=0}^{\infty} K^{N} [u(k)]^{N} = \sum_{N=0}^{\infty} K^{N} \sum_{n} e^{ikn} P(n,N)$$

$$P(k,N) = [u(k)]^{N} = \sum_{n} e^{ikn} p(n,N) \tag{17}$$

$$P(n,N)=\frac{1}{2\pi}\int_{-\pi}^{\pi}e^{ikn}[u(k)]^N dk=\frac{1}{2\pi}\int_{-\pi}^{\pi}e^{-ikn}\sum_{m=0}^{N}\binom{N}{m}p^m e^{ikm}q^{N-m}e^{-ik(N-m)}dk$$

If $\left(n-m+N-m=0,\ \ m=\frac{N+n}{2}\right)$ $\rightarrow$ The integral $\neq 0$

$$P(n,N)=\frac{N!}{\left(\frac{N+n}{2}\right)!\left(\frac{N-n}{2}\right)!}p^{\frac{N+n}{2}}q^{\frac{N-n}{2}} \qquad \textbf{(18)}$$

$\rightarrow$ CLT OK

* $\tilde{P}(k,K)$ **(15)** $\rightarrow$ $P(k,N)$ **(17)** $\rightarrow$ $P(n,N)$ **(18)**

$\boxed{*\ \tilde{P}(k,K)\ \textbf{(15)} \to \tilde{P}(n,K)\ \textbf{(14)} \to P(n,N)\ \textbf{(18)}}$

$$
\begin{array}{ccc}
P(n,N) & \longleftarrow & P(k,N) \\
\uparrow & & \uparrow \\
\tilde{P}(n,K) & \longleftarrow & \tilde{P}(k,K)
\end{array}
$$

$$\tilde{P}(k,K) = \sum_n e^{ikn}\tilde{P}(n,K)$$

$$= \sum_n e^{ikn} \sum_{N=0}^{\infty} K^N P(n,N)$$

$$\tilde{P}(n,K) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \tilde{P}(k,K)e^{-ikn}\,dk = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{dk\,e^{-ikn}}{1-Ku(k)}$$

$$\longrightarrow \quad \tilde{P}(n,K) = \frac{1}{\sqrt{1-4pqK^2}}\left[\frac{\sqrt{1-4pqK^2}}{2Kq}\right]^{|n|} \qquad \textbf{(19)}$$

$$\longrightarrow \quad P(n,N) = \frac{1}{2\pi i}\oint \frac{\tilde{P}(n,K)}{K^{N+1}}dk \quad \left(\tilde{P}(n,K) = \sum_{N=0}^{\infty} K^N P(n,N) \quad \to \textbf{(18)}\right)$$

§4. Master Equation

$$\begin{cases} \tau = unit\ hopping\ time = const \\ t = N\tau \end{cases} \tag{20}$$

($\tau \to 0,\ N \to \infty,\ N\tau \to const$ 가는 극한에서 ($t \to continuous$))

$$P(n,N) \Rightarrow P(n,t) \tag{21}$$

$$\frac{P(n,t) - P(n,t-\tau)}{\tau} = \frac{p}{\tau}P(n-1,t-\tau) + \frac{q}{\tau}P(n+1,t-\tau) - \frac{1}{\tau}P(n,t-\tau)$$

$$\boxed{\begin{aligned} \frac{dP(n,t)}{dt} &= \omega_- P(n-1,t) + \omega_+ P(n+1,t) - \omega_0 P(n,t) \\ &= \sum_{n'} W(n,n')P(n',t) \end{aligned}} \tag{22}$$

: (Master Equation)

Transition Rate
$$\begin{cases} W(n,n-1) = p/\tau = \omega_- \\ W(n,n+1) = q/\tau = \omega_+ \\ W(n,n) = -1/\tau = \omega_0 \\ W(n,n') = 0 \qquad (n' \neq n, n-1, n+1) \end{cases}$$

Fourier Transform ($k \leftrightarrow n$)

$$P(k,t) = \sum_n e^{ikn} P(n,t)$$

$$\frac{dP(k,t)}{dt} = \omega(k)P(k,t) \qquad (\ \omega(k) \equiv \omega_+ e^{ik} + \omega_- e^{-ik} - \omega_0\ ) \tag{23}$$

$$\begin{Bmatrix} P(n, t=0) = \delta_{no} \\ P(k, t=0) = 1 \end{Bmatrix} \rightarrow P(k,t) = e^{\omega(k)t} \tag{24}$$

$$\omega(k) = \omega_0(\cos k - 1) + 2i\delta\omega \sin k \qquad (\ 2\delta\omega \equiv \omega_+ - \omega_-\ )$$

$$P(k,t) = e^{\omega_0(\cos k - 1)t} e^{(2i\delta\omega \sin k)t}$$

$$P(k,t) = e^{-\omega_0 t} \sum_{l=-\infty}^{\infty} e^{ikl} I_l(\omega_0 t) \sum_{m=-\infty}^{\infty} (-i)^m e^{ikm} I_m(2i\delta\omega t) \tag{25}$$

(I_l : modified Bessel function)

comparing with $P(k,t) = \sum_n e^{ikn} P(n,t)$,

$$P(n,t) = e^{-\omega_0 t} \sum_{m=-\infty}^{\infty} (-i)^{n-m} \, I_m(\omega_0 t) I_{n-m}(2i\delta\omega t) \qquad \textbf{(26)}$$

<u>Non-biased(pure) RW</u> $(\delta\omega = 0)$

$$\rightarrow P(n,t) = e^{-t} I_n(t) \quad (\ \tau = 1, \omega_0 = 1\ ) \qquad \textbf{(27)}$$

$$P(n,t) \xrightarrow[t\,\rightarrow\,\infty]{n\,\rightarrow \text{fixed}} \frac{1}{\sqrt{2\pi \mathrm{t}}}\left[1 - \frac{4n^2-1}{8t} \ldots\right] \qquad \textbf{(28)}$$

cf) $\left\{ \begin{array}{c} \text{CLT Scaling} \\ \\ \left\{ \begin{array}{c} n \rightarrow \infty \\ t \rightarrow \infty \\ n^2/t \rightarrow \text{fixed} \end{array} \right\} \end{array} \right.$ $\quad P(n,t) = \dfrac{1}{\sqrt{2\pi t}} \exp\left(-\dfrac{n^2}{2t}\right)$

Laplace Transform $(s \to t)$

$$\tilde{P}(n,s) \equiv \int_0^\infty e^{-st} P(n,t)dt \quad (K \leftrightarrow e^{-s})$$

$$s\tilde{P}(n,s) - \tilde{P}(n,t=0) = \frac{1}{2}\tilde{P}(n+1,s) + \frac{1}{2}\tilde{P}(n-1,s) - \tilde{P}(n,s) \qquad \textbf{(29)}$$

From Master Equation of Pure RW ($p = q = \frac{1}{2}$, $\tau = 1$),

$$n \neq 0, \quad \tilde{P}(n,s) = a[\tilde{P}(n+1,s) + \tilde{P}(n-1,s)] \quad \left(a = \frac{1}{2(s+1)}\right) \qquad \textbf{(30)}$$

$$\tilde{P}(n,s) = A\lambda^n \quad (n > 0)$$

$$\tilde{P}(n,s) = A\lambda_-^n \quad \left(\lambda_- = \left(1 - \sqrt{1-4a^2}\right)/2a\right)$$

$$n = 0, \quad s\tilde{P}(0,s) - 1 = \frac{1}{2}\tilde{P}(1,s) + \frac{1}{2}\tilde{P}(-1,s) - \tilde{P}(0,s) = P(1,s) - P(0,s)$$

$$\tilde{P}(n,s) = \frac{1}{s+1-\lambda_-}\lambda_-^n \qquad \textbf{(31)}$$

$s \to 0$ (or long time limit $t \to \infty$) $\to \lambda_- \to (1 - \sqrt{2s}) \to \tilde{P}(n,s) \simeq \frac{(1-\sqrt{2s})^n}{\sqrt{2s}+s}$

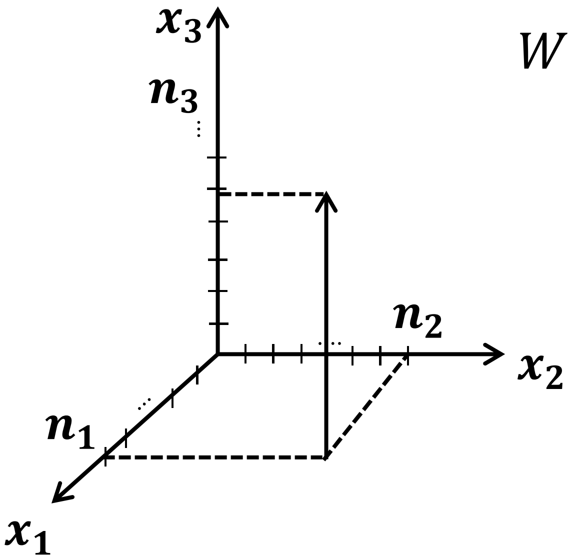
$$\tilde{P}(n,s) \xrightarrow{s \to 0} \frac{e^{-n\sqrt{2s}}}{\sqrt{2s}} \qquad \text{(Asymptotic formula)} \qquad \textbf{(32)}$$

$$P(n,t) = \int_{s_0 - i\infty}^{s_0 + i\infty} \tilde{P}(n,s) e^{st} ds \qquad \to \text{CLT}$$

Master Equation of RW on d-dimensional lattice

A lattice point $\vec{n}$:

$$\begin{cases} \vec{n} = (n_1, n_2, \dots, n_d) = n_1\hat{x}_1 + n_2\hat{x}_2 + \cdots + n_d\hat{x}_d \\ \hat{x}_i \text{ : unit lattice vector } (i = 1,2,\dots,d) \end{cases}$$



$$W(\vec{n},\vec{n}') = \frac{1}{z}\delta_{n_i,n_i'\pm 1} \qquad (\text{for } \forall\, i, z = 2d, \tau = 1) \qquad \textbf{(40)}$$

$$\frac{dP(\vec{n},t)}{dt} = \frac{1}{z}\sum_{i=1}^{2d}[(P((\dots,n_i+1,\dots);t) +(P((\dots,n_i-1,\dots),t)] - P(\vec{n};t) \qquad \textbf{(41)}$$

$$\frac{dP(\vec{n},t)}{dt} = \frac{1}{z}\sum_{\vec{n'}}\mathcal{L}_{\vec{n}\vec{n}'}P(\vec{n},t) \qquad \textbf{(42)}$$

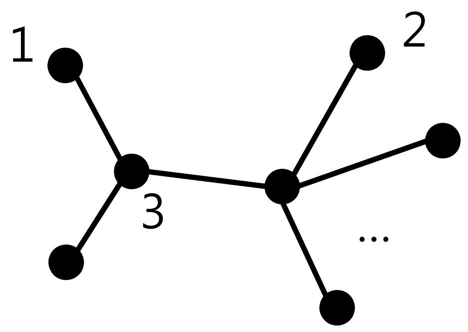
$$\frac{d\vec{P}}{dt} = \frac{1}{z}\overleftrightarrow{\mathcal{L}_L}\vec{P} \qquad \vec{P} = \begin{bmatrix} P(\vec{0}) \\ \vdots \\ P(\vec{n}) \\ \vdots \end{bmatrix} \tag{43}$$

$\overleftrightarrow{\mathcal{L}_L} = \{\mathcal{L}_{\vec{n}\vec{n}'}\}$: Lattice Laplacian

$$\overleftrightarrow{\mathcal{L}_L} = \begin{bmatrix} -z & \overbrace{1, 1, \ldots, 1,}^{\boldsymbol{z}} & & 0\ 0\ 0 \\ \vdots & \ddots & & \\ 0\ 0\ 0\ 1, & \overbrace{1, -z, 1, \ldots}^{\boldsymbol{z+1}} & 0\ 0\ 0 & \\ & & \ddots & \vdots \\ 0\ 0\ 0\ 0 & \ldots 1 & \overbrace{\ldots 1, 1,}^{\boldsymbol{z}} & 1, -z \end{bmatrix} \tag{44}$$

$\leftrightarrow \nabla^2$

Master Equation on Any graph



$A_{12} = 0$
$A_{13} = 1$
$\vdots$
$\{A_{mn}\}$ =Adjacency matrix

$$\frac{dP(m,t)}{dt} = \sum_n \frac{A_{mn}}{k_n} P(n,t) - k_m \frac{1}{k_m} P(m,t)$$

$$= \sum_n \left[\frac{A_{mn}}{k_n} - \delta_{mn} \right] P(n,t)$$

$$= \sum_n [A_{mn} - k_m \delta_{mn}] \frac{1}{k_n} P(n,t)$$

$$\frac{dP(m,t)}{dt} = \sum_n \sum_l [A_{mn} - k_m \delta_{mn}] \frac{\delta_{nl}}{k_l} P(l,t) \qquad \textbf{(45)}$$

$$\frac{d\vec{P}}{dt} = \overleftrightarrow{\mathcal{L}}_G \cdot \overleftrightarrow{D}^{-1} \vec{P} \qquad \left(\vec{P} = \begin{bmatrix} P_1 \\ \vdots \\ P_N \end{bmatrix} \right) \qquad \textbf{(46)}$$

$\overleftrightarrow{\mathcal{L}_G}$: Laplacian Matrix $\leftrightarrow \nabla^2$
graph Laplacian

$$\overleftrightarrow{\mathcal{L}_G} = \begin{pmatrix} -k_1, \overbrace{1,1, \dots, 1}^{k_1}, 0, \dots \\ \vdots \quad \ddots \\ \\ \dots, \overbrace{1,1, \dots 1}^{k_N}, -k_N \end{pmatrix} \tag{47}$$

$$\overleftrightarrow{D} = \begin{pmatrix} k_1, 0,0, \dots 0,0, \dots \\ \vdots \quad \ddots \\ \\ \dots, 0,0, \dots 0, k_N \end{pmatrix} \tag{48}$$

§5. Diffusion Equation

Discrete lattice → continuum space : $na \rightarrow x$

$$\frac{d}{dt}P(x,t) = \frac{p}{\tau}P(x-a,t) + \frac{q}{\tau}P(x+a,t) - \frac{1}{\tau}P(x,t)$$

$$\frac{d}{dt}P(x,t) = \frac{2a^2pq}{\tau}\left[\frac{P(x+a,t)+P(x-a,t)-2P(x,t)}{a^2}\right]$$
$$-\frac{a(p-q)}{\tau}\left[q\frac{P(x+a,t)-P(x,t)}{a} + \frac{P(x,t)-P(x-a,t)}{a}\right]$$

$$\boxed{\frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial x^2} - v\frac{\partial P}{\partial x}} \quad \begin{pmatrix} \tau \rightarrow 0, a \rightarrow 0 \\ D \rightarrow 2pqa^2/\tau, v = \dfrac{a}{\tau}(p-q) \end{pmatrix} \tag{33}$$

: (Drift−Diffusion Equation / Convection−Diffusion Equation)

Scaling Solution Ansatz

$$P(x,t) = \frac{1}{X(t)} f\left(\frac{x}{X(t)}\right) \quad \textbf{(34)}$$

(From normalization condition)

$$u = x/X(t)$$

$$X\dot{X} = -D\frac{f''(u)}{f(u) + uf'(u)} = A$$

$$\rightarrow P(x,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(\frac{-(x-vt)^2}{4Dt}\right) \qquad (\ P(x,0) = \delta(x)\ )$$

Fourier Transform ($x \leftrightarrow k$)

$$\int P(x,t)e^{ikx}dx = P(k,t)$$

$$\dot{P}(k,t) = (ikv - Dk^2)P(k,t)$$

$$P(k,t) = e^{i(kv-Dk^2)t} \quad \textbf{(35)}$$

(CLT 증명에서 $Q(k) \sim e^{ikm_1 - k^2 m_2/2}$)

$$\int P(k,t)e^{-kx}\,dk \ \rightarrow \text{CLT}$$

Laplace Transform ($t \leftrightarrow s$, $K \leftrightarrow e^{-s}$)

$$\tilde{P}(x,s) = \int_0^\infty e^{-st} P(x,t)dt$$

$$s\tilde{P}(x,s) - \delta(x) + v\tilde{P}(x,s) = D\frac{\partial \tilde{P}(x,s)}{\partial x^2}$$

$$\tilde{P}(x,s) = \frac{1}{\sqrt{v^2+4Ds}} e^{-\alpha_\pm(s)|x|} \qquad \left(\alpha_\pm(s) = \frac{v \pm \sqrt{v^2+4sD}}{2D}\right) \tag{36}$$

$$P(x,t) = \int_{s_0-i\infty}^{s_0+i\infty} \tilde{P}(x,s)e^{st}ds \;\rightarrow\; \text{CLT}$$

Fourier-Laplace Transform

$$\tilde{P}(k,s) = \int_{-\infty}^{\infty} dx\, e^{ikx} \int_0^\infty e^{-st}\, dt\, P(x,t) = \frac{1}{s+ivk+Dk^2} \tag{37}$$

In d dim. ,

$$\frac{\partial P(\vec{r},t)}{\partial t} = D\nabla^2 P(\vec{r},t) - \vec{v}\cdot\nabla P(\vec{r},t) \qquad (\ \vec{v} = const\ )$$

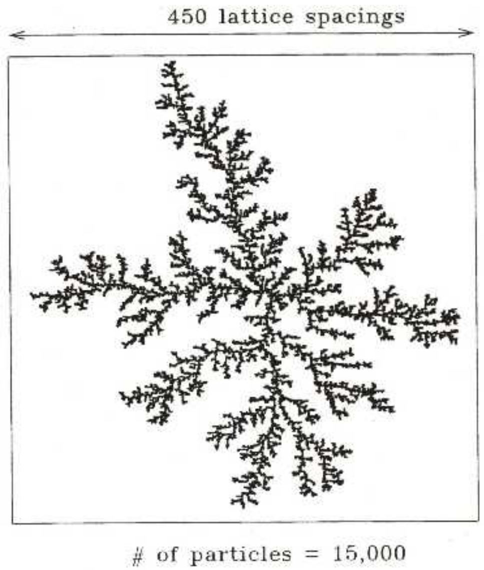
$$= D\nabla^2 P(\vec{r},t) - \nabla\cdot(P(\vec{r},t)\vec{v}) \tag{38}$$

$$P(\vec{r},t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{(\vec{r}-\vec{v}t)^2}{4Dt}\right) \qquad (\ \vec{P}(\vec{r},0) = \delta(\vec{r})\ ) \tag{39}$$

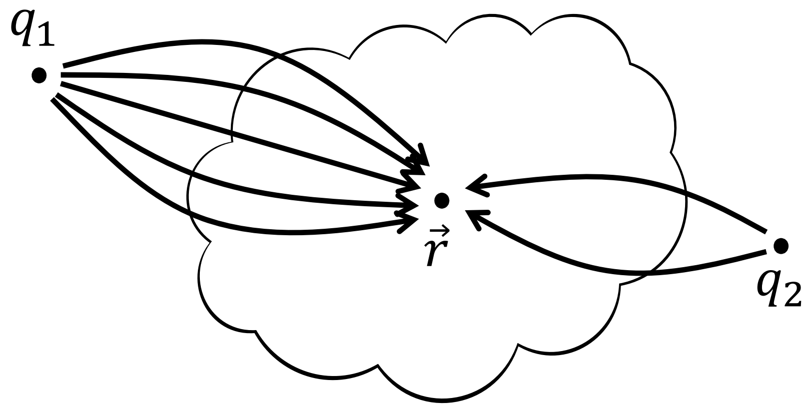
Laplace Equation ↔ Electrostatics Analogy

$$\left(\frac{dP}{dt} = \nabla^2 P, \qquad \frac{dP}{dt} = 0, \qquad \nabla^2 P = 0\right)$$

1. Application : Laplacian growth
   → Diffusion limited aggregation



2. Laplace Equation의 RW solution (charge → <u>RW source</u>)



$$\begin{cases} q_1 > q_2 : \text{No. of RW starting from } q_1 \text{ is larger than that of from } q_2. \\ P(\vec{r}) \sim \Phi(\vec{r}) : \text{No. of RWs arriving at } \vec{r}. \end{cases}$$

§4. RWs on finite systems (graph)

(Exercise) Prove the following theorem

on Master equation $\left(\frac{dP(m,t)}{dt} = \sum_{n'} W(n,n')P(n',t)\right)$.

① There is at least one stationary solution for $\frac{dP(m)}{dt} = \dot{P}(m) = 0$.

② This stationary solution is unique when the graph G in which a pair $\{n,n'\}$ with $W(n,n') \neq 0$ is connected is a connected graph.

③ If $0 \leq P(n,0) \leq 1$ for $\forall\, n$ at $t=0$, and $\sum_n P(n,0) = 1$, then $0 \leq P(n,t) \leq 1$ and $\sum_n P(n,t) = 1$ at $\forall\ t > 0$.

④ Set $P(n,t) = a_n \exp(-\lambda t)$. Then the master equation yields a set of linear equation for $\{a_n\}$, with eigenvalue λ. λ's have the following property.

a) The real part of λ is nonnegative : $\mathrm{Re}\lambda \geq 0$.

b) If the detailed balance holds or $W(n,n')P(w') = W(n',n)P(n)$ λ is real and $\lambda \geq 0$.

⑤ If the stationary solution is unique, $\{P(n,t)\}$ with any initial condition $\{P(n,0)\}$ tends to the stationary solution in the limit $t \to \infty$.

$\boxed{P(\vec{n}, t) \text{ on d-hyper cubic lattice}}$

From the theorem on Master Equation and Lattice Laplacian,

$$\rightarrow P(\vec{n}, t) = \sum_{\alpha=0} a_\alpha(\vec{n}) e^{-\lambda\alpha t}$$

1) $\lambda_\alpha \geq 0$

2) Especially $\overleftrightarrow{\mathcal{L}_L}$ has always null eigenvalue($\lambda_0 = 0$) with the eigenvector $\{a_0(\vec{n}) = \frac{1}{L^d}\}$, which is the stationary state ($t \rightarrow \infty$).

3) λ_1 (2nd smallest eigenvalue) decides final transient behavior.

RWs on finite graphs

From (27), $\frac{d\vec{P}}{dt} = \overleftrightarrow{\mathcal{L}_G} \cdot \overleftrightarrow{D}^{-1}\vec{P}$,

$\overleftrightarrow{\mathcal{L}_G}$ has null eigenvector $(\lambda_0 = 0)$ $\rightarrow$ $\left[\overleftrightarrow{D}^{-1}\vec{P}\right] = \begin{bmatrix} 1/N \\ 1/N \\ \vdots \\ 1/N \end{bmatrix}$

$P_0(m) \propto cD_m \propto ck_m$

$$P_0(m) = \frac{k_m}{\sum k_m} = \frac{k_m}{2N\langle k\rangle} \quad \text{(Professor Noh's centrality)} \qquad \textbf{(49)}$$

* Professor Noh's statement

① RW in the steady state traverses any link with the equal probability.

② RW in the steady state thus stays a certain node with the probability proportional to its degree.