- **Chapter 3. Variants of random walk**

(Main Refs. [3], [*])

§ 1. Lévy flights.

§ 2. Walks with memory.

§ 3. Continuous time R.W.

§ 4. Generating function and RG.

§ 1. Levy flights (walks)

CLT 의 조건 중 philosophy 2 가 깨지는 경우

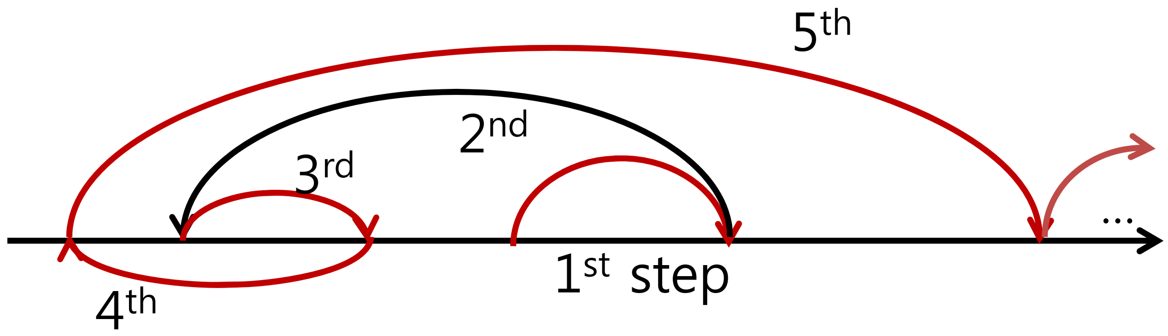
$$* \; \langle u \rangle = \int p(u) u = m, \qquad \langle u \rangle^2 = \int p(u)\, u^2$$

등이 존재하지 않는 경우 중

<u>$p(u)$가 power-law를 만족하는 경우</u>

→ Lévy flight(walk) (LF)

1d 에서

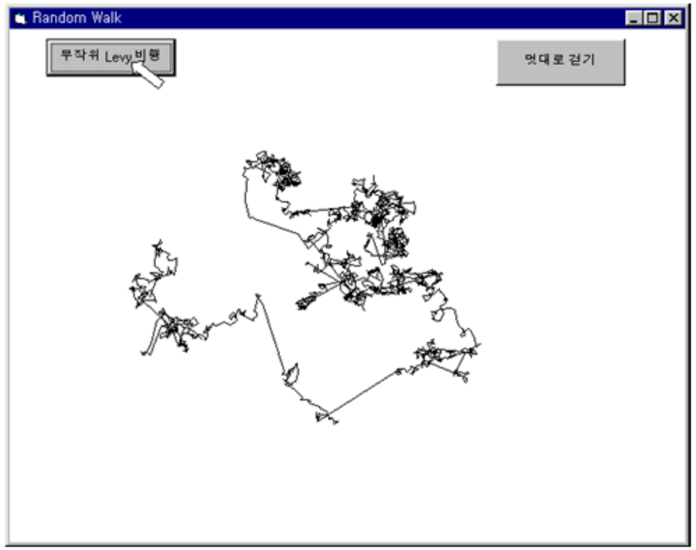


$$p(u) = \frac{1}{c} u^{-(1+\eta)} \quad (\eta > 0) \qquad \textbf{(1)}$$

① $\eta > 2 \rightarrow m_1, m_2$ exists
CLT → satisfied **(2)**

② $1 < \eta < 2\,, m_2$ or $\langle u \rangle^2$ diverges.
CLT → unsatisfied **(3)**

③ $0 < \eta < 1,$ both m_1 and m_2 diverge.
CLT → unsatisfied **(4)**



PDF of $R = u_1 + u_2 + \cdots + u_n$

$$u_m(N) = \max(u_1, u_2, \ldots, u_m) \tag{5}$$

$$N\int_{u_m(N)}^{\infty} p(u)du \; = 1 \rightarrow u_m(N) \approx N^{1/\eta} \tag{6}$$

$$\rightarrow p(u \gg u_m(N), N) = 0$$

* Biased LF for $0 < \eta < 1$

$$R = N\int_0^{u_m(N)} up(u)du = \begin{cases} N^{1/\eta} & (\eta < 1) \\ N \ln N & (\eta = 1) \end{cases} \tag{7}$$

* LF for $1 < \eta \leq 2$

$$(\Delta R)^2 = (R - \langle R \rangle)^2 = N \int_0^{u_m} (u - m_1)^2 p(u) du = \begin{cases} N^{2/\eta} & : 1 < \eta < 2 \\ N \ln N & : \eta = 2 \end{cases} \quad \textbf{(8)}$$

$(\langle R \rangle = N m_1), (d_L$: fractal time of LF)

$$\underline{d_L = \eta}$$

* LF scaling

$$p(N,R) = \begin{cases} N^{-\frac{1}{\eta}} f\left(\frac{R}{N^{\frac{1}{\eta}}}\right) & (0 < \eta < 1) \\ N^{-\frac{1}{\eta}} f\left(\frac{R - \langle R \rangle}{N^{\frac{1}{\eta}}}\right) & (1 < \eta < 2) \end{cases} \quad \textbf{(9)}$$

* LF on 2d, 3d space → Eqs. **(7)**, **(8)**, **(9)**, OK.

(Exercise) Prove **(9)** by simulation [(cf) (1-12)].

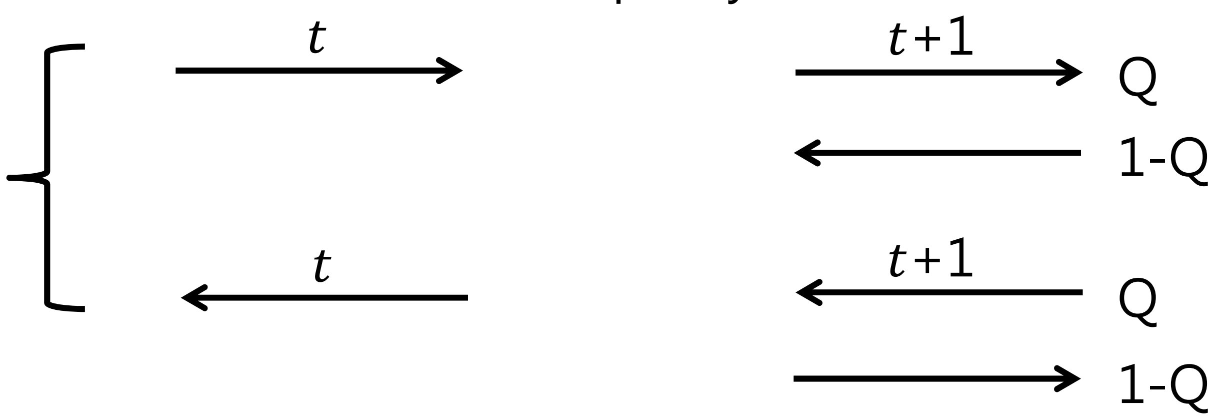
§ 2. Walks with memory

Break the philosophy 3 of CLT

Memory or interaction effect

① Persistent RW

Consider 1d RW for simplicity



Walker has the tendency to move in the same direction as it moved at previous time → Markovian process of the second order

$$\begin{cases} L(N;n) \text{ : the prob. that a walker arrives at } n \text{ after } N \text{ steps with the last step takes the left direction.} \\ R(N;n) \text{ : the prob. that a walker arrives at } n \text{ after } N \text{ steps with the last step takes the right direction.} \end{cases}$$

Recursion relation

$$\begin{aligned} L(N+1;n) &= QL(N;n+1) + (1-Q)R(N;\mathrm{n}+1) \\ R(N+1;n) &= QR(N;n+1) + (1-Q)L(N;\mathrm{n}+1) \end{aligned} \qquad \textbf{(10)}$$

$$P(n,N) \approx \sqrt{\frac{1-Q}{2\pi NQ}} \exp\left[-n^2 \frac{1-Q}{2NQ}\right] \qquad \textbf{(11)}$$

Persistent length : $\ell_p = \sum_{\ell=1}^{\infty} \ell Q^{\ell}(1-Q) = \frac{Q}{1-Q} = N_p$ **(12)**

Rescaling the number of step (time scale)

$$N' = \frac{N}{\ell_p} = \frac{N}{N_p}$$

$$P(n, N) \approx \sqrt{\frac{1}{2\pi N'}}\exp[-\frac{n^2}{2N'}] \qquad \textbf{(13)}$$

→ Simple RWs

(Exercise) Prove Eq. **(11)**
(Exercise) From the persistent random walks, Show

[Telegraph Equation]

$$\frac{\partial R(x,t)}{\partial t} + v\frac{\partial R(x,t)}{\partial x} = \gamma\big(L(x,t) - R(x,t)\big)$$

$$\frac{\partial L(x,t)}{\partial t} + v\frac{\partial L(x,t)}{\partial x} = \gamma\big(R(x,t) - L(x,t)\big)$$

By taking a continuous limit of space time

② Self-avoiding walks (SAWs)

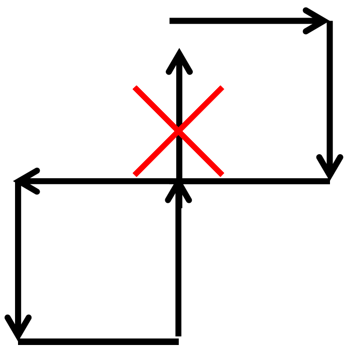
Polymer in good solvent

Isolated (diluted) polymer

Break the philosophy 3

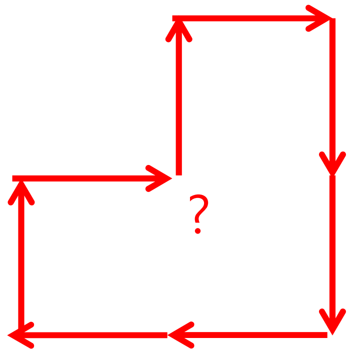
→ Non-Markovian walks
(Excluded volume effects)
(Repulsive interactions between monomers)

→ Walker cannot visit the already-visited sites, bonds, points, etc.



SAWs on lattices

1st theoretical version : Growing SAWs → Dead end problem



→ True self-avoiding walks?

2nd theoretical version : Ensemble of N-step walks (N-SAWs)

Consider 2nd version first

$\mathcal{J}_N \sim N^{\gamma-1}\mu^N$: # of possible N-SAWs **(1-9)**

* μ : Effective coordination number

$\mu \leq z-1$ (z : coordination number of the lattice)

$R_E^2 \equiv \langle R^2 \rangle \sim N^{2\nu}$ (end-to-end distance). **(1-7)**

$$R_g^2 \equiv \frac{1}{N}\left\langle \sum_{i=1}^{N}\left(\overrightarrow{u_i}-\overrightarrow{R_i}\right)^2 \right\rangle \ \left(\overrightarrow{R_i}=\frac{1}{N}\sum_{i=1}^{N}\overrightarrow{u_i}\right)$$

$\sim N^{2\nu}$ (radius of gyration)

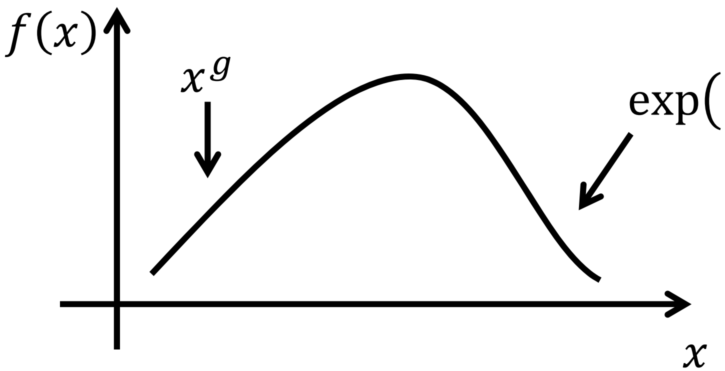
$(d_{SAW} = \frac{1}{\nu})$

Essential properties of SAWs

① $P(R,N) = \frac{\mathcal{J}_N^{SAW}(R)}{\mathcal{J}_N^{SAW}} \approx \frac{1}{R_E^d} f\left(\frac{R}{R_E}\right)$ **(14)**

(scaling property)

$1/R_E^d$ ~ Normalization $[\int d^d R \; P(R,N) = 1]$

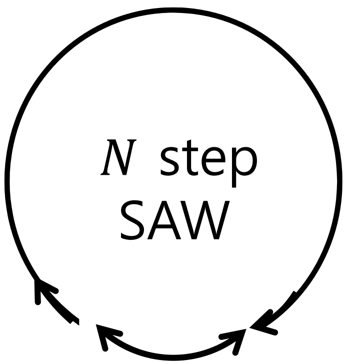


$$f(x) \approx x^g \exp(-x^\delta) \quad \textbf{(15)}$$

$$\delta \approx (1-\nu)^{-1} \quad \textbf{(16)}$$

(By the mapping to $n = 0$ n-vector model)

②



$$\mathcal{J}_N^{SAW}(R = a) \approx \mu^N \left(\frac{a}{R_E}\right)^d \quad \textbf{(17)}$$

(From uniform distribution of end points in the volume of R_E^d)

$$P(a,N) = \frac{1}{R_E^d}\left(\frac{a}{R_E}\right)^g \approx \frac{1}{R_E^d} N^{-\nu g} \qquad \textbf{(18)}$$

$$P(a,N) = \frac{\mathcal{J}_N^{SAW}(a)}{\mathcal{J}_N^{SAW}} \approx \frac{1}{R_E^d} N^{1-\gamma} \qquad \textbf{(19)}$$

$g = \frac{\gamma-1}{\nu}$ (des Cloiseaux relation) **(20)**

From Eqs **(16)**, **(20)** → (γ,ν) → (γ,ν,δ,g)
(Ref. [6]: Chapter 1)

Flory approximation

Free energy of polymers

$$F = E - TS$$

① E : Repulsive interaction between monomer → Mean-field energy

$\left(\rho = \frac{N}{R^d} : \text{monomer density}\right)$

Effective range of repulsive interaction : ℓ

ϵ : the energy for a pair of monomers

$$E_{re} = \epsilon N \rho \ell^d = \ell^d \epsilon \frac{N^2}{R^d} = C_{re} \frac{N^2}{R^d} \qquad \textbf{(21)}$$

② Entropy term (S)

$$
\begin{aligned}
S_N(R) &\approx \ln \mathcal{J}_N(R) \\
&\approx \ln p(N,R)\,\mathcal{J}_N \quad \left(\because\, p(N,R) = \frac{\mathcal{J}_N(R)}{\mathcal{J}_N}\right)
\end{aligned}
$$

[Pure RW]

$$
\begin{aligned}
&\approx \ln \exp\left(-\left(\frac{R^2}{N}\right)\right)\mathcal{J}_N \\
&\approx \ln \mathcal{J}_N - C\,\frac{R^2}{N} \qquad \textbf{(22)}
\end{aligned}
$$

$$-TS = E_{el} = const. + C\,\frac{R^2}{N} \qquad \textbf{(23)}$$

(Elastic energy of polymer)

$$F = E - TS$$
$$= C_{re}\frac{N^2}{R^d} + C_{el}\frac{R^2}{N} + const \qquad \textbf{(24)}$$

$$\frac{\partial F}{\partial R} = 0 \ \rightarrow \nu_F = \frac{3}{d+2} \ \ (R_E \sim N^{\nu}) \qquad \textbf{(25)}$$

$$\frac{1}{d_{SAW}} = \nu_F = \begin{cases} 1 & (d=1) \\ 3/4 & (d=2) \\ 3/5 & (d=3) \\ 1/2 & (d=4) \end{cases} \begin{pmatrix} \nu_{\mathrm{ex}} = 1 \\ \nu_{\mathrm{ex}} = 3/4 \\ \nu_{\mathrm{ex}} = 0.58 \\ \nu_{\mathrm{ex}} = 1/2 \end{pmatrix} \qquad \textbf{(26)}$$

* ν_F is an amazing result considering the crude approximation of E_{el} & E_{re}.

* E_{re} is overestimated due to the repulsion.

* $E_{el} \sim -TS \ \rightarrow \ S_{rw} > S_{SAWs}$

* Two overestimates of E_{el} & E_{re} interfere constructively
→ ν_F is a relatively exact result.

* $d \geq 4$: $\nu_F = \nu_{SAW} = \frac{1}{2}$ $(d_w = d_{SAW} = 2)$

$$E_{re}^{SAW} \leq E_{re}^{max} = C_{re}\frac{N^2}{R_{RW}^d} \approx C_{re}N^{2-\frac{d}{2}} \quad \textbf{(27)}$$

E_{re}^{max} is neglible if $d > 4$
(Excluded volume effect is negligible)

($d_u = 4$: upper critical dimension)
($d_l = 1$: lower critical dimension)

→ reminiscence of n-vector (Ising) model

Mapping to $n = 0$ n-vector model

* n-vector model : classical model of ferromagnetism.

$$\mathcal{H} = -J\sum_{\langle ij\rangle} \vec{S_i}\cdot\vec{S_j}\left(-h\sum_i \vec{S_i}\right) \qquad \textbf{(28)}$$

$$\underline{\left|\vec{S_i}\right|^2 = 1, \vec{S_i} = (S_i^1, S_i^2, \ldots, S_i^n) = \{S_i^\alpha\}}$$

$n \to 0$ 에서

$$\langle S^\alpha(0) S^\alpha(R)\rangle\Big|_{n\to\infty} = \sum_N \mathcal{J}_N^{SAW}(R) K^N \quad \left(K = \frac{J}{k_B T}\right) \qquad \textbf{(29)}$$

$G(K,R) = \sum_N \mathcal{J}_N^{SAW}(R) K^N \rightarrow$ generating function of walk models
(K : fugacity)

(Exercise) Prove **(29)**

Susceptibility

$$\chi = \sum_R \langle s^\alpha(0) s^\alpha(R)\rangle \Big|_{n\to 0} = \sum_R \sum_N \mathcal{J}_N^{SAW}(R) K^N$$

(Fluctuation-Dissipation theorem)

$$= \sum_N \mathcal{J}_N^{SAW} K^N = \sum_N (K\mu)^N N^{\gamma-1} \qquad \textbf{(30)}$$

$$\begin{cases} K_c \approx \frac{1}{\mu} \text{ (Convergence radius)} \\ \text{or } T_c = J\mu/k_B \end{cases} \qquad \textbf{(31)}$$

$$\begin{cases} \frac{T-T_c}{T} \equiv \bar{t} \text{ (Reduced temp.)} \\ \bar{t} \to 0 \text{ (Critical regime)} \end{cases}$$

$$K - K_c \approx -K_c \bar{t} \to K = K_c \exp(-\bar{t})$$

$$\chi \equiv \sum_N \exp(-N\bar{t})\, N^{\gamma-1} \approx \int_0^\infty \exp(-N\bar{t})\, N^{\gamma-1}\, dN$$

$$\chi \approx \bar{t}^{-\gamma} \qquad \textbf{(32)}$$

$$C(R) = \langle S^{\alpha}(0) S^{\alpha}(R) \Big|_{n\to 0} = \sum_N \mathcal{J}_N^{SAW}(R) K_c^N \exp(-N\bar{t})$$

$$= K_c^N \int_0^{\infty} dN \mathcal{J}_N^{SAW}(R) \exp(-N\bar{t}) \qquad \textbf{(33)}$$

$$\begin{cases} \text{Laplace transform of } \mathcal{J}_N^{SAW}(R) \to C(R) \\ (N \leftrightarrow \bar{t}) \to \text{conjugate variables} \end{cases}$$

(Exercise) Prove that $\delta = (1-\nu)^{-1}$ **(16)** from

$$C(R) \approx \frac{\exp\left(-\frac{R}{\xi}\right)}{R^{d-2+\eta}}$$

and

$$\xi \sim \bar{t}^{-\nu}$$

by using **(33)** and . $P(R,N) \approx \frac{\mathcal{J}_N^{SAW}(R)}{\mathcal{J}_N^{SAW}}$

$$\langle S^{\alpha}(0)S^{\alpha}(a)\rangle\Big|_{n\to 0} = \sum_{N} K_c^N \mathcal{J}_N(a)\exp(-N\bar{t})$$

$$\varepsilon_s = -\frac{1}{2}zJ\langle S(0)S(a)\rangle$$ (ε_s: Exchange energy per spin)

$$\approx \int dN\, \mathcal{J}_N(a)\exp(-N\bar{t})$$

$$\approx \bar{t}^{(1-\alpha)} \quad \left(\frac{\partial \varepsilon_S}{\partial \bar{t}} = C_{heat} = \bar{t}^{-\alpha}\right)$$

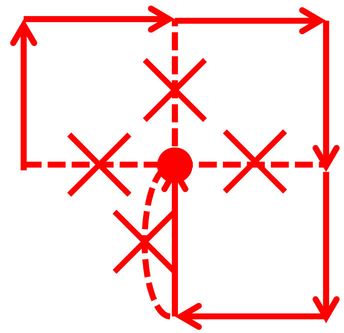
$\mathcal{J}_N(a) \approx N^{\alpha-2} \approx N^{-\nu d} \approx \dfrac{1}{R_E^d}$ → Eq. (**17**) (∵hyper scaling $\alpha = 2 - \nu d$)

Consider now growing version of walk models : 1st version

* Survival probability of SAWs at N-step.

$$\approx S(N) = \frac{\mathcal{J}_N^{SAW}}{\mathcal{J}_N^{RW}} \approx N^{\gamma-1} \left(\frac{\mu}{z}\right)^N$$

* Dead end → no more growth

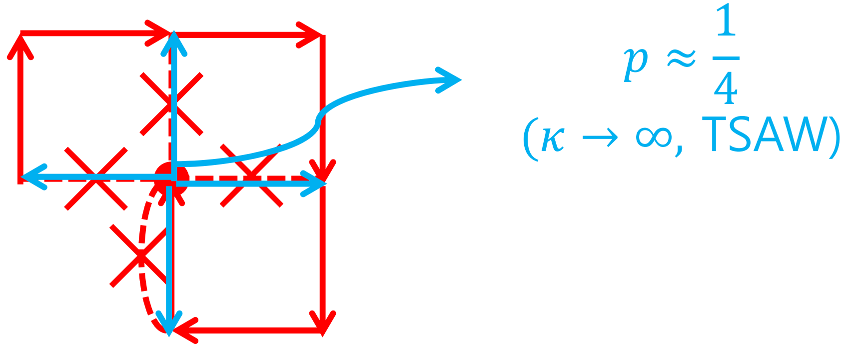


To circumvent the dead end. → True self-avoiding walks (TSAWs)

$$p(\vec{R}, \vec{R}+\vec{\delta}) = \frac{e^{-\kappa n\left(\vec{R}+\vec{\delta}\right)}}{\sum_{\vec{\delta}} e^{-\kappa n\left(\vec{R}+\vec{\delta}\right)}} \quad \textbf{(34)}$$

: hopping probability to one of the nearest neighbor $\vec{\delta}(\in \{\vec{a_i}\}: i = 1, \dots, 2d)$

$n(\vec{R}+\vec{\delta})$: the number that the walk has visited the site $\vec{R}+\vec{\delta}$.



$$\nu_{TSAW} = \frac{2}{d+2}\left(d_{TSAW} = \frac{d+2}{2}\right) = \begin{cases} \frac{2}{3} & : d = 1 \\ 2 & : d \geq 2 \quad (d_u = 2) \end{cases} \quad \textbf{(35)}$$

(Exercise) Study the following walk models and investigating the critical properties by simulation.

① growing self-avoiding walks
(kinetic growth walks)
② Indefinitely growing SAWs
③ Trail (Θ- collapse)
④ Hamiltonian walk
⑤ Directed (Anisotropic) walk

Final remarks

* Ballistic motion $\nu_B = 1$

$$\left(\nu_B \geq \nu_{any}\right)$$

* Super diffusion $\left(\nu > \frac{1}{2}\right)$

* Sub diffusion $\left(\nu < \frac{1}{2}\right)$

§ 3. Continuous time R.W.

Break the philosophy ①: RW can take variable time interval between hops (steps) or RW can sit on a site for a considerable time before leaving.

→ continuous time RWs.

$q(t)dt$: the probability that RW leaves site at the time between t and $t + dt$ after arriving the site.

$a(\tau)$: The probability that RW does not take the step up to τ.

$$a(\tau) = \prod_{i=1}^{m} (1 - q(t_i)dt_i) \quad \left(dt_i = \frac{\tau}{m}\right)$$

$$a(\tau) = \prod_{i=1}^{m} \left(1 - q(t_i)\right) dt_i = \exp\left[\sum_{i=1}^{m} \ln\left(1 - q(t_i)\right) dt_i\right]$$

$\boxed{dt_i \to 0}$

$$= \exp\left(-\sum_{i=1}^{m} q(t_i) dt_i\right)$$

$$a(\tau) = \exp\left(-\int_0^{\tau} q(t) dt\right) \tag{36}$$

* $a(\infty) \to 0$, if $\int_0^{\infty} q(t)dt \to \infty$

RW leaves the site any-way.

* $a(\infty) \to$ finite, if $\int_0^{\infty} q(t)dt =$ finite

RW has a finite probability to stay the site eternally.

Then, the prob. that RW leaves the site at the interval $(t_1, t + dt_1)$

$$\rightarrow a(t_1)q(t_1)dt_1 \tag{37}$$

Thus, the prob. that RW leaves the site

$$\begin{aligned}
&\rightarrow \int_0^\infty a(t_1)q(t_1)dt_1 = \int_0^\infty \exp\left[-\int_0^{t_1} q(t)dt\right] q(t_1)dt_1 \\
&= -\exp\left[-\int_0^{t_1} q(t)dt\right]\Big|_0^\infty \\
&= a(0) - a(\infty) \\
&= 1 - a(\infty)
\end{aligned} \tag{38}$$

Furthermore, the prob. that RW takes a step at the time interval $(t_1, t_1 + dt_1)$ to a site with the relative position $(\vec{r}, \vec{r} + d\vec{r})$ is

$$p(\vec{r}, t) = q(t_1)p(\vec{r})dt\, d^d r. \quad \textbf{(39)}$$

Then $P(r,t) \propto \exp\left(-\frac{Br^2}{2m_2 t}\right) \quad (m_1 = 0)$ **(40)**

$$\propto \exp\left(-\frac{r^2}{2m_2 \bar{t}}\right)$$

$$\left(\bar{t} = \frac{t}{B}, B = \int_0^\infty a(t)dt\,, \text{(time−rescaling)}\right)$$

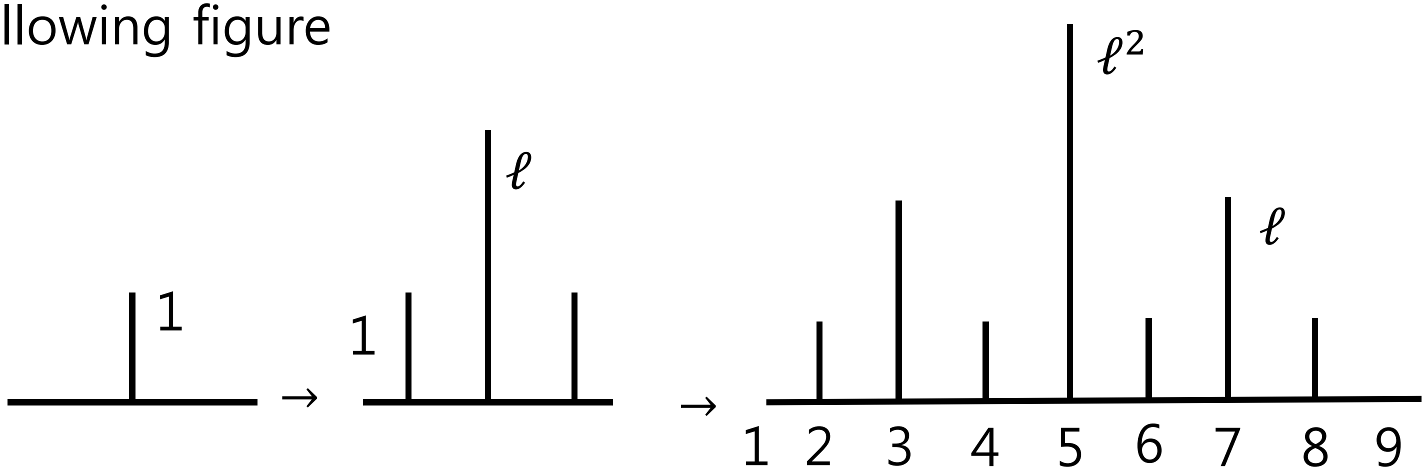
(Exercise) Prove (40) by using Laplace and Fourier transforms.

Anomalous effects comes when $p(\vec{r}, t$ is not separable as in Eq. (**39**)

(Exercise)

i) Find $P(n,t)$on a regular comb with the sidebranches of length ℓ that are spaced at unit intervals on a backbone of linear chain.

ii) Find $P(n,t)$on the bifurcating hierarchical comb like the following figure



§ 4. Generating function and Renormalization group

$$G(K) = \sum_{N=1}^{\infty} \mathcal{J}_N K^N \qquad \left(\mathcal{J}_N = \sum_R \mathcal{J}_N(R) \right) \qquad \textbf{(41)}$$

(K : fugacity ($\mathcal{J}_N \sim \mu^N N^{\gamma-1}$))

$$\begin{cases} G(K) \text{ converges if } \mu K < 1 \\ K_c = \frac{1}{\mu} \end{cases} \qquad \left(K\mu = \frac{K}{K_c} \right)$$

$$K\mu = 1 - \frac{K_c - K}{K_c} = 1 - \bar{K} \qquad \left(\bar{K} \equiv \frac{K_c - K}{K_c} \right)$$

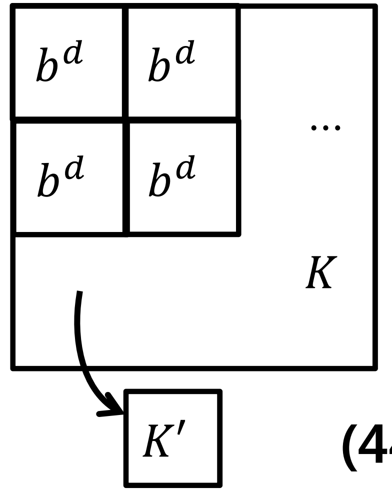
$$G(K) = \int_0^{\infty} K^N \mu^N N^{\gamma-1}\, dN \approx \int_0^{\infty} \exp(-\overline{K}N)\, N^{\gamma-1}\, dN \qquad \textbf{(42)}$$

$$G(K) \approx \overline{K}^{-\gamma} \qquad \textbf{(43)}$$

$$R_E(N) = \langle R^2 \rangle^{\frac{1}{2}} \sim N^{\nu}$$

$$\langle R_E \rangle_K = \frac{\sum_N R_E(N) N^{\gamma-1} (\mu K\ )^N}{G(K)} \approx \overline{K}^{-\nu}$$

Real space renormalization group of $G(K)$ (RSRG)



Consider b^d-size cell,

$$\to G_b(K) = \textstyle\sum_{N=1}^{b} \mathcal{J}_N K^N = K' \qquad \textbf{(44)}$$

RS Renor.

$$K^* = G_b(K^*) \qquad \textbf{(45)}$$

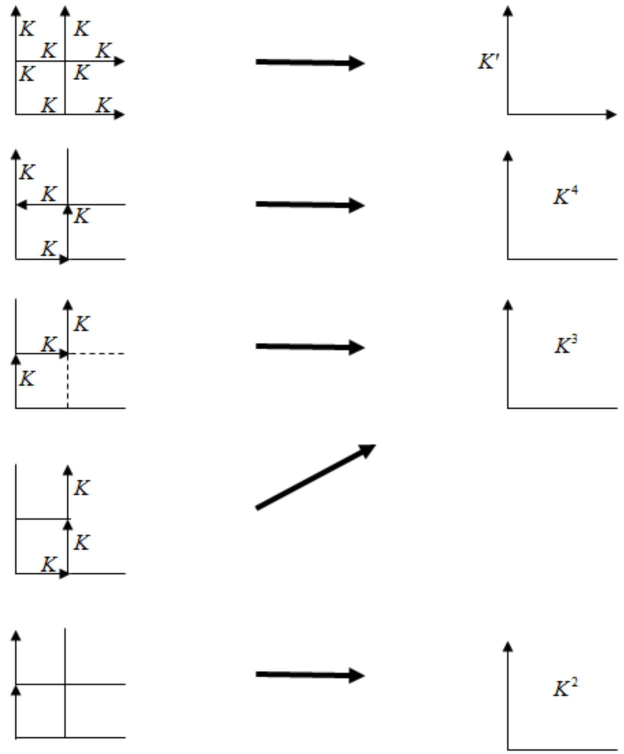
$K^* \to$ fixed point

$$\underline{K^* \equiv K_c} \qquad \textbf{(46)}$$

$$\begin{aligned} K' &= G_b(K^*) + \left.\frac{dG_b}{dK}\right|_{K^*} (K - K^*) \\ &= K^* + \left.\frac{dG_b}{dK}\right|_{K^*} (K - K^*) \end{aligned} \qquad \textbf{(47)}$$

$$\langle R_E \rangle_K \approx (K^* - K')^{-\nu} = b^{-1}(K^* - K)^{-\nu} \qquad \textbf{(48)}$$

$$\boxed{\nu = \frac{\ln b}{\ln \lambda} \qquad \left(\lambda = \left.\frac{dG_b}{dK}\right|_{K^*}\right)} \qquad \textbf{(49)}$$



Small cell RG of SAWs (Example)

$\rightarrow b = 2$

(corner law) $\longrightarrow$ $K' = K^2 + 2K^3 + K^4$

$K^* = 0,\ 0.379$

$K^* = 0.379 \rightarrow \nu \approx 0.72 \left(\nu_{\text{ex}} = \frac{3}{4}\right)$

Crude approximation

Large cell Monte Carlo RG

$\rightarrow$ Needed