- **Chapter 2. First Passage Problems.**

(Main Refs. [2], [4])

§1. Introduction.

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§4. $F(\vec{r} = 0, t \to \infty)$. First Passage Prob. to Origin.

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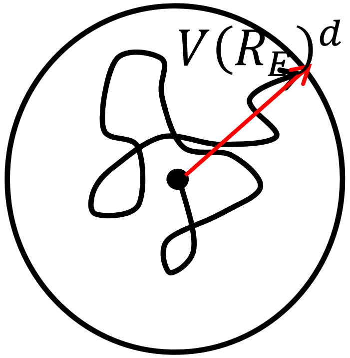
§7. Electrostatics and Hitting prob.

§1. Introduction

$\begin{cases} \text{i) Upper critical dimension of RWs?} \\ \text{ii)} \begin{cases} \text{Reentrant(Recurrent) RW?} \\ \text{Transparent RW? (transient)} \end{cases} \end{cases}$

$$\begin{cases} V \sim (R_E)^d \sim N^{\frac{d}{2}} \\ \text{No. of hoppings } \sim N \end{cases}$$



If $V < N$, RW covers V compactly & completely→ Recursive (Reentrant).
$(d < 2)$

If $V > N$, RW covers V partly → Transparent (Transient).
$(d > 2)$

$\boxed{d_c = 2}$?

Main Physical Quantities of interests

① First Passage Probability
$F(\vec{r}, t)$: Prob. that RW visits $\vec{r}$ for the first time at t.

② No. of distinct visited sites : $\mathcal{D}(t)$

③ $O(\vec{r}, t)$: Occupancy of $\vec{r}$ by RW up to t
No. of visits of RW to $\vec{r}$ up to t

§2. First Passage Probability

$F(\vec{r},t) \leftrightarrow P(\vec{r},t)$

$$P(\vec{r},t) = \delta_{\vec{r}0}\delta_{t0} + \sum_{t' \le t} F(\vec{r},t')P(0,t-t') \quad \textbf{(1)}$$

$$\tilde{P}(\vec{r},K) = \sum_{t=0}^{\infty} K^t P(\vec{r},t), \qquad \tilde{F}(\vec{r},K) = \sum_{t=0}^{\infty} K^t F(\vec{r},t) \quad \textbf{(2)}$$

$$\tilde{P}(\vec{r},K) = \delta_{\vec{r}0} + \tilde{F}(\vec{r},K)\tilde{P}(0,K)$$

$$\tilde{F}(\vec{r},K) = \frac{\tilde{P}(\vec{r},K) - \delta_{\vec{r}0}}{\tilde{P}(0,K)} = \begin{cases} \dfrac{\tilde{P}(\vec{r},K)}{\tilde{P}(0,K)}; \vec{r} \neq 0 \\ 1 - \dfrac{1}{\tilde{P}(0,K)}; \vec{r} = 0 \end{cases} \quad \textbf{(3)}$$

§3. Laplace Transform and Real time Quantities

$$f(t) \leftrightarrow \tilde{f}(K) = \sum_{t=0}^{\infty} f(t) K^t$$

The relation singular behavior of $f(t)$ to $\tilde{f}(K)$

Main Re.

$$\begin{aligned} &\tilde{f}(K) \sim (1-K)^{\mu-1} \qquad (\mu < 1) \\ &\qquad (\simeq \infty (K \to 1\text{-})) \\ &\to f(t) \sim t^{-\mu} \qquad (t \to \infty) \end{aligned} \tag{4}$$

$$\tilde{f}(K) = \sum_{t=0}^{\infty} f(t) K^t = \int^{\infty} f(t) e^{-t \ln(1/K)}\, dt \simeq \int^{t^*} f(t) dt \quad (t^* = [\ln(1/K)^{-1}]) \tag{5}$$

$$\left(\tilde{f}(K) = \tilde{f}(s) \text{ (Laplace Transform) } \left(s = \ln(1/K) \right) \right) \tag{6}$$

$\therefore s \to 0 \ \left(\ln(1/K) \Rightarrow 0, K \to 1 \right) \to$: long time limit ($= \tilde{f}(K \to 1\text{-})$)

$\therefore \sum_{t=0}^{\infty} f(t)$ (diverges) $\to$ cutoff t^* $\to$ Asymptotic behavior at $t \to \infty$

$\boxed{\text{a) The case in which } \sum_{t=0}^{\infty} f(t)\left(= \tilde{f}(K = 1\text{-})\right) \text{ diverges}}$

$$\begin{cases} K \to 1, \qquad s \to 0, \qquad s = \ln(1/K) = 1 - K \\ \hline t^* = [\ln(1/K)]^{-1} = \dfrac{1}{1-K} \approx 1/s \end{cases} \tag{7}$$

$$\tilde{f}(K) = \int^{s^{-1}} f(t)dt \tag{8}$$

$$= \int^{s^{-1}} t^{-\mu}dt \sim s^{\mu-1} \sim (1-K)^{\mu-1} \qquad (K \to 1\text{-})$$

$\boxed{\text{* Diverging } \tilde{f}(k = 1\text{-}) \leftrightarrow \left(f(t) \sim t^{-\mu} \ \to\ \tilde{f}(K) \sim (1-K)^{\mu-1} \right) \qquad (\mu < 1)}$

* Useful Relation ①

$$P(t) = \sum_{t'=0}^{t} f(t') \tag{9}$$

$$\rightarrow \ \tilde{P}(K) = \frac{\tilde{f}(K)}{1-K} \tag{10}$$

And, $P(t) = \int_0^t f(t')dt$

$$\tilde{P}(s) = \tilde{f}(s)/s \qquad (\ 1 - K = s\ ) \tag{11}$$

* Useful Relation ②

$$\left.\begin{aligned} P(t) &= \int_0^t f(t')dt' \\ \tilde{f}(K) &= \int_0^{t^*} f(t')dt' \\ &= \int_0^{1/s} f(t')dt' \end{aligned}\right\} P(t^*) = \tilde{f}(K = 1 - s) = \tilde{f}\left(K = 1 - \frac{1}{t^*}\right) \tag{12}$$

b) The case in which $\sum_{t=0}^{\infty} f(t)\left(=\tilde{f}(K=1)\right)$ converges

No cutoff is needed

* $f(t) \sim t^{-\mu} \quad (\mu > 1)$

($\tilde{f}(K=1)$ is finite)

$$\tilde{f}(K) = \tilde{f}(1) - p_1(1-K)^{\alpha_1} + \cdots \qquad (K \to 1) \tag{13}$$

$$\tilde{f}(1) - \tilde{f}(K) \propto p_1(1-K)^{\alpha_1}$$

$$\propto \sum_t t^{-\mu}(1-K^t) \quad \sim \int^{\infty} t^{-\mu}(1-e^{-st})dt \qquad \left(\because s = \frac{1}{\ln K}\right)$$

$$\sim \int_{1/s}^{\infty} t^{-\mu} dt$$

$$\tilde{f}(1) - \tilde{f}(K) \sim (1/s)^{-\mu+1} \sim (1-K)^{\mu-1} \tag{14}$$

$$\tilde{f}(K) \sim \tilde{f}(1) - a_1(1-K)^{\mu-1} + \cdots \tag{15}$$

§4. $F(\vec{r}=0, t\to\infty)$: First Passage Prob. to origin.

$P(\vec{r}=0,t)=(4\pi Dt)^{-d/2}$ (Pure RW)

$$\tilde{P}(0,K) \simeq \int^{\infty} K^t P(0,t)dt$$

$$\simeq \int_0^{\infty} (4\pi Dt)^{-d/2} K^t dt \qquad \textbf{(16)}$$

As expected, $\tilde{P}(0,K=1)$ diverges when $d \le 2$

→ singular property : case a)

$\tilde{P}(0,K=1)$ converges when $d > 2$

→ singular property : case b)

i) $d \le 2$

$$\tilde{P}(0,K) \propto \int^{t^*} (4\pi Dt)^{-\frac{d}{2}} dt$$

$$\sim \begin{cases} A_d (t^*)^{1-d/2} = A_d (1-K)^{d/2-1} & ;\ d<2 \quad \text{(Eq. (7))} \\ A_2 \ln t^* = -A_2 \ln(1-K) & ;\ d=2 \end{cases} \qquad \textbf{(17)}$$

ii) $d > 2$

($\tilde{P}(0, K = 1) = \int^{\infty} P(0, t) dt$ converges)

$$\tilde{F}(0, K = 1) = \sum_t F(0, t) = 1 - [\tilde{P}(0, K = 1)]^{-1} \quad \text{(From Eq. (3))} \quad \textbf{(18)}$$

$R = \tilde{F}(0, K = 1)$: Eventual Prob. that RW reaches the origin.

$$\tilde{P}(0, K = 1) = [1 - R]^{-1} \quad \textbf{(19)}$$

From Eq. (13) and $K = 1 - s$,

$$\begin{aligned} \tilde{P}(0,1) - \tilde{P}(0, K) &\propto \sum_t t^{-d/2}(1 - K^t) \\ &= (1 - K)^{d/2-1} \end{aligned} \quad \textbf{(20)}$$

$$\tilde{P}(0, K) \sim (1 - R)^{-1} + B_d (1 - K)^{\frac{d}{2}-1} + \cdots \qquad (d > 2) \quad \textbf{(21)}$$

From Eq. (3), $\tilde{F}(0,K) = 1 - \dfrac{1}{\tilde{P}(0,K)}$,

(d = 1), $\tilde{P}(0,K) = (1-K)^{-\frac{1}{2}}$

$$\tilde{F}(0,K) = 1 - \sqrt{1-K} \tag{22}$$

$$\tilde{F}(0,K) = \begin{cases} 1 - \dfrac{1}{A_d(1-K)^{d/2-1}} & : d < 2 \\ 1 + \dfrac{1}{A_2 \ln(1-K)} & : d = 2 \\ R + B_d(1-R)^2(1-K)^{\frac{d}{2}-1} & : d > 2 \end{cases} \tag{23}$$

$$\tilde{F}(0,1-1/t^*) \sim \int_0^{t^*} F(0,t)dt$$

= first passage probability up to t^*

$$= T(t^*) = 1 - S(t^*) \qquad \textbf{(24)}$$

($S(t^*)$: survival prob. up to t^*)

$$S(t) = \begin{cases} \dfrac{1}{A_d t^{1-d/2}} & : d < 2 \\[2ex] \dfrac{1}{A_2 \ln t} & : d = 2 \\[2ex] 1 - R + B_d (1-R)^2 t^{1-d/2} & : d > 2 \end{cases} \qquad \textbf{(25)}$$

$$F(0,t) = -\frac{\partial S(t)}{\partial t} \propto \begin{cases} t^{d/2-2} & : d < 2 \\[2ex] \dfrac{1}{t \ln^2 t} & : d = 2 \\[2ex] t^{-d/2} & : d > 2 \end{cases} \qquad \textbf{(26)}$$

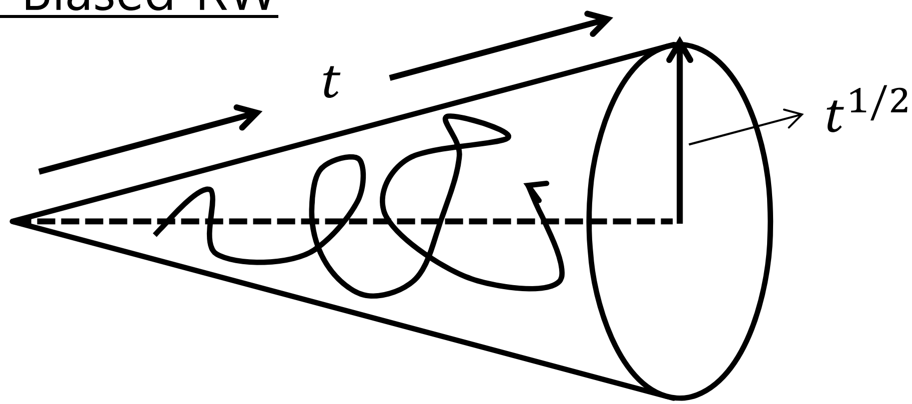
$$
* \begin{cases} \langle t \rangle = \int tF(0,t)dt \\ R = \int F(0,t)dt = 1 \\ \boxed{\lim_{t\to 0} S(t) \to 0} \end{cases}
\begin{pmatrix} \text{diverges } d < 2 \\ \\ d < 2 \end{pmatrix}
$$

$$
\to \begin{pmatrix} \text{Reentrant} \\ \text{Recurrent} \end{pmatrix} \text{RW } (d < 2)
$$

$$
\begin{cases} \underline{\text{Compact Exploration}} \\ \text{RW visits any site infinitely many times} \end{cases}
$$

* $d > 2$ $R(S)$ is finite. Transient (Transparent) RW

<u>* Biased RW</u>



$$V \sim t \cdot t^{\frac{d-1}{2}} \sim t^{\frac{d+1}{2}}$$

$$\rho \sim \frac{t}{t^{\frac{d+1}{2}}} \sim t^{\frac{1-d}{2}}$$

$d > 1$: Transparent

(Exercise) 1차원 pure RW가 위치 x에 처음 도달 확률 $F(x,t)$는

$$F(x,t) = x \cdot \frac{t^{-3/2}}{\sqrt{4\pi D}} \exp(-x^2/4Dt)$$

임을 보여라.

(hint) i) $\tilde{P}(x,s) = \tilde{P}(x-x',s)F(x',s)$

$$\left(\tilde{P}(x,s) = \int ds\, e^{-st} P(x,t) \right)$$

ii) Eq. (34)

§5. No. of distinct visited sites : $\mathscr{D}(t)$

$$\mathcal{D}(t) = tS(t) \sim \begin{cases} t^{\frac{d}{2}} & : d < 2 \\ \dfrac{t}{\ln t} & : d = 2 \\ (1-R)t + \cdots & : d > 2 \end{cases} \qquad \textbf{(27)}$$

$$\mathcal{D}(t) = 1 + \sum_{\vec{r}\neq 0} \{F(\vec{r},1) + F(\vec{r},2) + \cdots + F(\vec{r},t)\}$$
$$\mathcal{D}(0) = 1,\ \mathscr{D}(1) = 2 \qquad \textbf{(28)}$$

$$\Delta(t) \equiv \mathcal{D}(t) - \mathcal{D}(t-1)$$
$$\Delta(1) = 1 \qquad \textbf{(29)}$$

$$\Delta(t) = \sum_{\vec{r}\neq 0} F(\vec{r},t) = -F(0,t) + \sum_{\vec{r}} F(\vec{r},t) \qquad \textbf{(30)}$$

$$\widetilde{\Delta}(K) = \sum_t K^t \Delta(t) \;\; = -\tilde{F}(0,K) + \sum_{\vec{r}} \tilde{F}(\vec{r},K)$$

From Eq. (3), $\tilde{F}(\vec{r},K) = \dfrac{\tilde{P}(\vec{r},K) - \delta_{\vec{r}0}}{\tilde{P}(0,K)}$ and $\sum_{\vec{r}} P(\vec{r},t) = 1$,

$$\widetilde{\Delta}(K) = -1 + \frac{1}{(1-K)\tilde{P}(0,K)} \tag{31}$$

$$\mathcal{D}\;(t) = \Delta(0) + \Delta_1 + \cdots + \Delta(t) \tag{32}$$

$$\widetilde{\mathcal{D}}(K) = \sum_t K^t \mathcal{D}(t) = \sum_{t=0}^{\infty} K^t \left(\sum_{l=0}^{t} \Delta(l) \right) = \frac{1}{1-K}[1 + \widetilde{\Delta}(K)]$$

$$\widetilde{\mathcal{D}}(k) = \frac{1}{(1-K)^2 \widetilde{P}(0,K)} \tag{33}$$

From Eq. (1-19), $\tilde{P}(0,K) = \dfrac{1}{\sqrt{1-K^2}}$ for 1d pure random walk

$$\widetilde{\mathcal{D}}(K) = \frac{\sqrt{1-K^2}}{(1-K)^2} = \frac{\sqrt{(1+K)(1-K)}}{(1-K)^2}$$

$K \to 1$-

$$= 2(1-K)^{-\frac{3}{2}} \simeq (1-K)^{\mu-1}$$

$$= \sum_{t=0}^{\infty} K^t \mathcal{D}(t) \qquad \textbf{(34)}$$

$$\mathcal{D}(t) \sim t^{-\mu} \sim t^{1/2} \quad \left(\text{Exactly, } \mathcal{D}(t) \overset{t\to\infty}{\sim} \sqrt{\frac{8t}{\pi}}\right) \text{ (1d} \to \text{Eq. (27))} \qquad \textbf{(35)}$$

* 2d, 3d → Eq. (27)

§6. First Passage Problem in an Interval

Interval : $x \in [0, L]$

* $\underline{P(0,t) = P(L,t) = 0}$: two absorbing boundaries.

$$\int_0^L P(x, t = 0)dx = 1$$

$$\rightarrow S(t) = \int_0^L P(x,t)dx < 1 \quad (?) \tag{36}$$

① Direct Solution of Diffusion Eq.

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

[cf) Free−Particle Schrödinger Equation

$$i\hbar\frac{\partial\phi}{\partial\tau} = -\frac{\hbar^2}{2m}\frac{\partial^2\phi}{\partial x^2}$$

$$\tau = -it, D = \frac{\hbar}{2m}$$

→ A particle in a box]

$$P(x,t) = \sum_{n=1}^{\infty}\frac{2}{L}\sin\left(\frac{n\pi x}{L}\right)e^{-\left(\frac{n\pi}{L}\right)^2 Dt} \quad \textbf{(37)}$$

$t \to \infty$

$$\begin{cases} S(t) \propto e^{-\left(\frac{\pi}{L}\right)^2 Dt} = e^{-\lambda_1 Dt} \ (\ \lambda_0 = 0\ ) \\ \\ \tau_1 = \dfrac{1}{\lambda_1 D} = \dfrac{L^2}{D\pi^2} \end{cases} \quad \textbf{(38)}$$

① Using Laplace Transform

$$s\tilde{P}(x,s) - P(x,t=0) = D\,\frac{d^2\tilde{P}(x,s)}{dx^2} \tag{39}$$

$$P(x,t=0) = \delta(x-x_0) \quad (x_0 \in [0,L])$$

$$\tilde{P}(x,s) = A\exp\left(x\sqrt{s/D}\right) + B\exp\left(-x\sqrt{s/D}\right) \tag{40}$$

with $P(0,t) = P(L,t) = 0$ and $P(x,t=0) = \delta(x-x_0)$

$$\tilde{P}(x,s) = \frac{\sinh\left(\sqrt{\frac{s}{D}}\,x_<\right)\sinh\left(\sqrt{\frac{s}{D}}\,(L-x_<)\right)}{\sqrt{sD}\,\sinh\left(\sqrt{\frac{s}{D}}\,L\right)} \tag{41}$$

$$\begin{pmatrix} x_> = \max(x,x_0) \\ x_< = \min(x,x_0) \end{pmatrix}$$

$$* \quad j_B = -D \left.\frac{\partial P(x,t)}{\partial x}\right|_{x_B} \tag{42}$$

(Diffusive current to boundary at x_B : prob. rate to hit the boundary.)

$$* \quad \mathcal{E}(x_B) = \int_0^{\infty} j(x_B, t)dt \tag{43}$$

(Eventual hitting prob. to x_B)

$$\tilde{P}(x,s) = \int_0^{\infty} e^{-st} P(x,t)dt \tag{44}$$

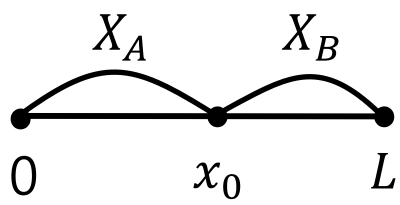
$$-D\frac{\partial \tilde{P}(x,s)}{\partial x} = \tilde{j}(x,s) = -D\frac{\partial}{\partial x}\int_0^{\infty} e^{-st} P(x,t)dt = \int_0^{\infty} e^{-st} j(x,t)dt \tag{45}$$

$$\tilde{j}(x,0) = \mathcal{E}(x) = \int_0^{\infty} j(x,t)dt \tag{46}$$

$$\begin{cases} \tilde{J}(x=0,s) = D\,\dfrac{\partial \tilde{P}(x,s)}{\partial x}\bigg|_{x=0} = \dfrac{\sinh\left(\sqrt{\dfrac{s}{D}}\,(L-x_0)\right)}{\sinh\left(\sqrt{\dfrac{s}{D}}\,L\right)} \\[2em] \tilde{j}(x=L,s\ ) = -D\,\dfrac{\partial \tilde{P}(x,s)}{\partial x}\bigg|_{x=L} = \dfrac{\sinh\left(\sqrt{\dfrac{s}{D}}\,x_0\right)}{\sinh\left(\sqrt{\dfrac{s}{D}}\,L\right)} \end{cases} \tag{47}$$

$$\begin{cases} \mathcal{E}(x=0) = \tilde{j}(x=0,s=0) = 1 - \dfrac{x_0}{L} \\ \mathcal{E}(x=L) = \tilde{j}(x=L,s=0) = \dfrac{x_0}{L} \end{cases} \tag{48}$$

$$* \quad \begin{cases} \mathcal{E}(0) = \dfrac{X_B}{X_A + X_B} \\ \mathcal{E}(L) = \dfrac{X_A}{X_A + X_B} \end{cases} \tag{49}$$



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

$$= \int_0^\infty \left(1 - st + \frac{s^2 t^2}{2!} + \cdots\right) j(x_B, t) dt$$

$$= \mathcal{E}(x_B)\left[1 - s\langle t(x_B)\rangle + \frac{s^2}{2!}\langle t(x_B)^2\rangle + \cdots\right] \quad \left(\mathcal{E}(x_B) = \int_0^\infty j(x_B, t) dt\right) \quad \textbf{(50)}$$

$$\langle t^n(x_B)\rangle = \frac{\int_0^\infty t^n(x_B) j(x_B, t) dt}{\mathcal{E}(x_B)} \quad \textbf{(51)}$$

$$\tilde{j}(0, s) = \left(1 - \frac{x_0}{L}\right)\left[1 - s\,\frac{2Lx_0 - x_0^2}{6D} + \cdots\right]$$

$$\tilde{j}(L, s) = \frac{x_0}{L}\left[1 - s\,\frac{L^2 - x_0^2}{6D} + \cdots\right]$$

$$\langle t(0)\rangle = \frac{2Lx_0 - x_0^2}{6D}$$

$$\langle t(L)\rangle = \frac{L^2 - x_0^2}{6D} \quad \textbf{(52)}$$

Mean Exit time : $\langle t_m \rangle$

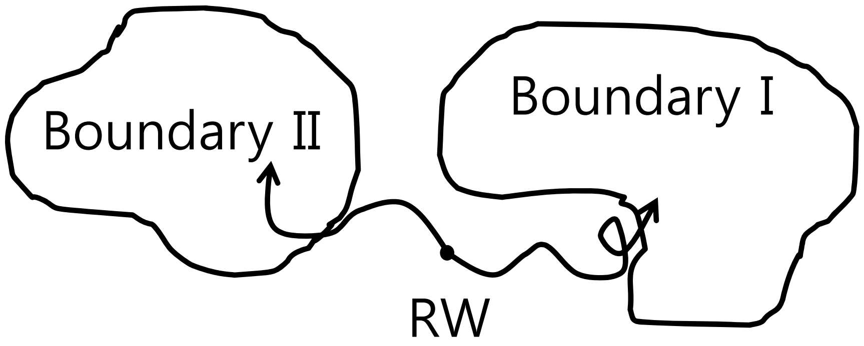
$$\begin{aligned}\langle t_m \rangle &= \mathcal{E}(0)\langle t_0 \rangle + \mathcal{E}(L)\langle t(L) \rangle \\ &= \frac{1}{2D} x_0 (L - x_0) \\ &= \frac{L^2}{D} u_0 (1 - u_0) \quad \left(u_0 = \frac{x_0}{L}\right) \\ &\propto \frac{L^2}{D} (u_0 \rightarrow \text{finite})\end{aligned} \tag{53}$$

$$\langle t_N \rangle \propto L \qquad \left(\text{if } \begin{array}{l} u_0 \rightarrow 0 \\ u_0 \rightarrow 1 \end{array}\right) \tag{54}$$

(Exercise) Consider this problem with one absorbing boundary and one reflecting boundary.

(Exercise) Consider this problem for biased random walk.

§7. Electrostatics and hitting prob.



$$j(\vec{r},t) = -D\hat{n}\cdot\vec{\nabla}P\Big|_{\vec{r}_B}$$

$$\mathcal{E}(\vec{r}_B) = \int_0^\infty j(\vec{r}_B,t)dt$$

From diff. Eq.,

$$P(\vec{r},t\to\infty) - P(\vec{r},t=0) = D\nabla^2\int_0^\infty dtP(\vec{r},t)$$

$$\begin{cases} P(\vec{r},t\to\infty)\to 0 \\ P(\vec{r},t=0) = \delta(\vec{r}-\vec{r}_0) \end{cases}$$

$$\mathcal{P}_0(\vec{r}) = \int_0^\infty dtP(\vec{r},t)dt$$

$$\nabla^2\mathcal{P}_0(\vec{r}) = -\frac{1}{D}\delta(\vec{r}-\vec{r}_0) \qquad \textbf{(55)}$$

* Laplace (Poisson Equation) for the single charge $\dfrac{1}{D\Omega_d}$ at $\vec{r}_0$

$$\mathcal{E}(\vec{r}_B) = \int_0^{\infty} j(\vec{r}_B, t)dt = -D\int \quad \hat{n}\cdot\nabla P(\vec{r},t)\Big|_{\vec{r}_B} dt$$

$$\mathcal{E}(\vec{r}_B) = -D\,\hat{n}\cdot\nabla P_0(\vec{r})\Big|_{\vec{r}_B} \qquad \textbf{(56)}$$

$$\langle t^n\rangle = \int_0^{\infty} t^n F(t)dt \; = -\int_0^{\infty} t^n \frac{\partial S(t)}{\partial t}dt$$

$$= n\int_0^{\infty} t^{n-1}\int_V \; P(\vec{r},t)d\vec{r} \qquad \textbf{(57)}$$

$$\mathcal{P}_n(\vec{r}) = \int_0^{\infty} P(\vec{r},t)t^n dt$$

$$\langle t^n\rangle = n\int_V \; \mathcal{P}_{n-1}(\vec{r})d\vec{r} \qquad \textbf{(58)}$$

$$\nabla^2\mathcal{P}_0(\vec{r}) = -\frac{1}{D}\delta(\vec{r}-\vec{r}_0)$$

$$\nabla^2\mathcal{P}_1(\vec{r}) = -\frac{1}{D}P_0(\vec{r}) \qquad \textbf{(59)}$$

$$\nabla^2\mathcal{P}_n(\vec{r}) = -\frac{n}{D}P_{n-1}(\vec{r})$$