Capture of particles and the distribution of the maximum of a random walk

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- Asymptotic properties of random walks

continuum limit → diffusion equation

- Finite size corrections?
  - relevant for physics (chemical reactions)
  - related with fluctuation theory

↓

universality in out of equilibrium systems

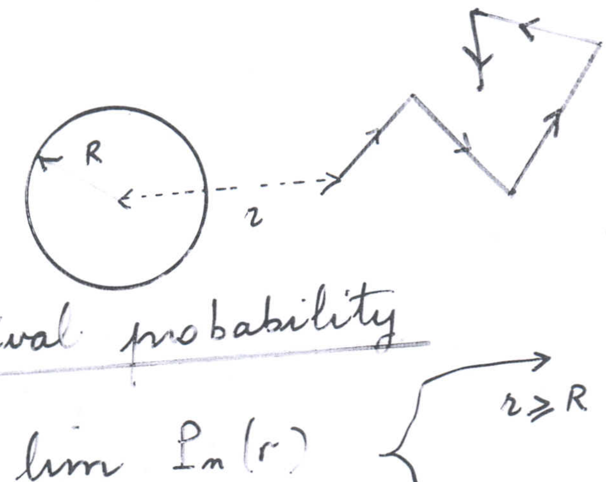
Problem I

- Expected maximum of a n step 1 d random walk

$$E(M_n) = \sigma\sqrt{\frac{2n}{3\pi}} - A + O\left(\frac{1}{\sqrt{n}}\right)$$

Problem II

- 3 d random walk with a spherical trap



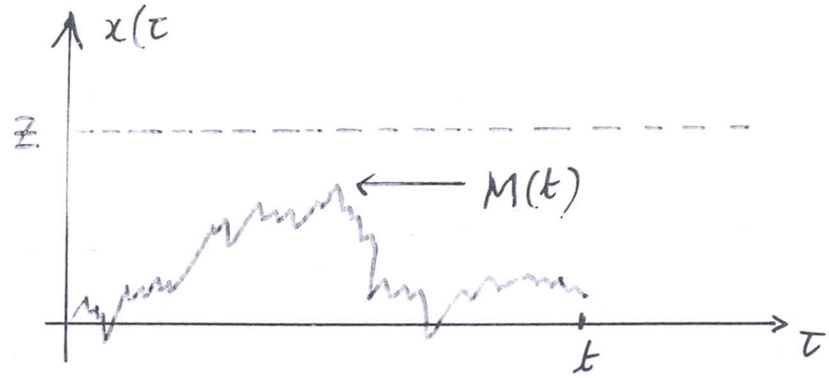
- survival probability

$$\lim_{n\to\infty} P_n(r) \begin{cases} \xrightarrow{r \gg R} & 1 - \dfrac{R - A'}{r} \\ \xrightarrow{r \to R} & B\,\dfrac{\sigma}{R} \end{cases}$$

$$A = A' = -\frac{1}{\pi}\int_0^\infty \frac{dk}{k^2}\log\left(\frac{1-\hat{f}(k)}{\sigma^2 k^2/2}\right) \qquad B = \frac{1}{\sqrt{2}}$$

Problem I

Expected maximum of a 1 d Brownian motion



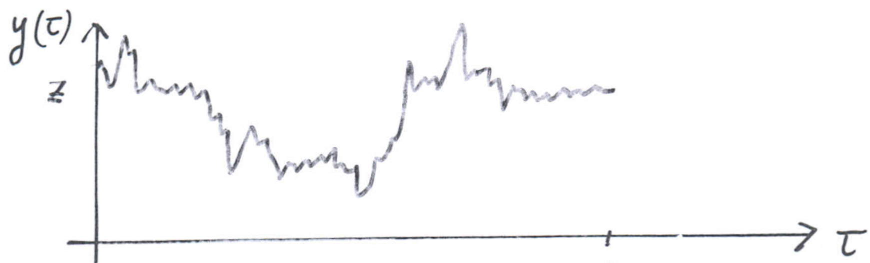
. $x(\tau)$ 1 d Brownian motion

. $E\,[x(\tau)x(\tau')] = 2D\min(\tau,\tau')$

. Maximum $\quad M(t) = \max\limits_{0\leq\tau\leq t} x(\tau)$

. $Q(z,t) = \text{Prob}\,[M(t) < z]$

. Path transformation $\quad x(\tau) \to y(\tau) = z - x(\tau)$



. $Q(z,t) = \text{Prob}\,[\,y(\tau) > 0 \mid y(0) = z\,]$
$\qquad\qquad 0 \leq \tau \leq t$

. Backward Fokker-Planck equation

$$\frac{\partial Q}{\partial t} = D\,\frac{\partial^2 Q}{\partial z^2}\,, \quad z \geq 0 \qquad \begin{cases} Q(z=0,t) = 0 \quad \forall t \\ Q(z,t=0) = 1 \\ \quad z \geq 0 \end{cases}$$

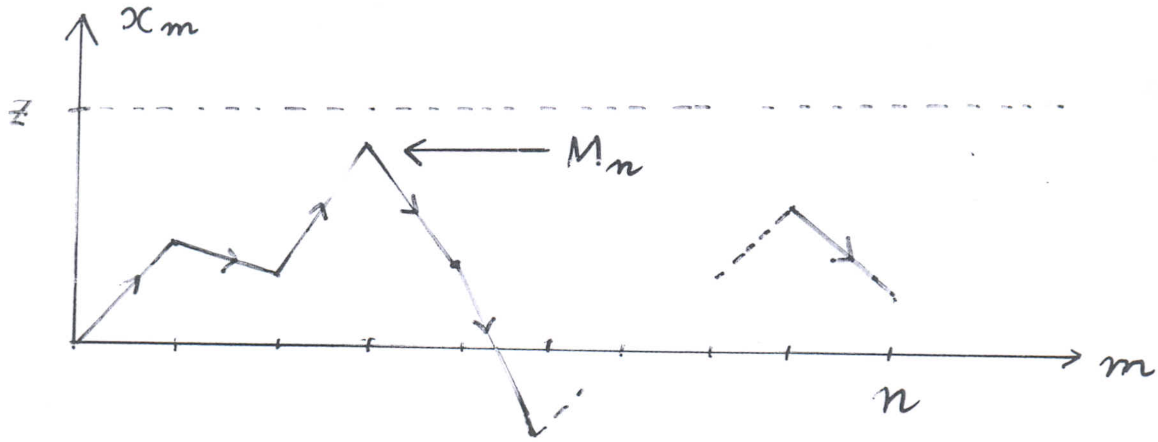
$\ldots(t) = |x(t)|$

$$\text{Prob}\,[M(t) < z] = Q(z,t) = \frac{2}{\sqrt{\pi}} \int_0^{\frac{z}{\sqrt{4Dt}}}$$

- Expected maximum

$$E(M(t)) = \int_0^\infty z \,\frac{\partial Q}{\partial z}(z,t)\, dz = \sqrt{\frac{4Dt}{\pi}}$$

1 d discrete time continuous space random walk



$$x_m = x_{m-1} + \xi_m \quad , \quad x_0 = 0$$

ξ_m : iid random variables

$$\text{Prob}\,[\xi_m \leq x] = \int_{-\infty}^{x} f(y)\, dy$$

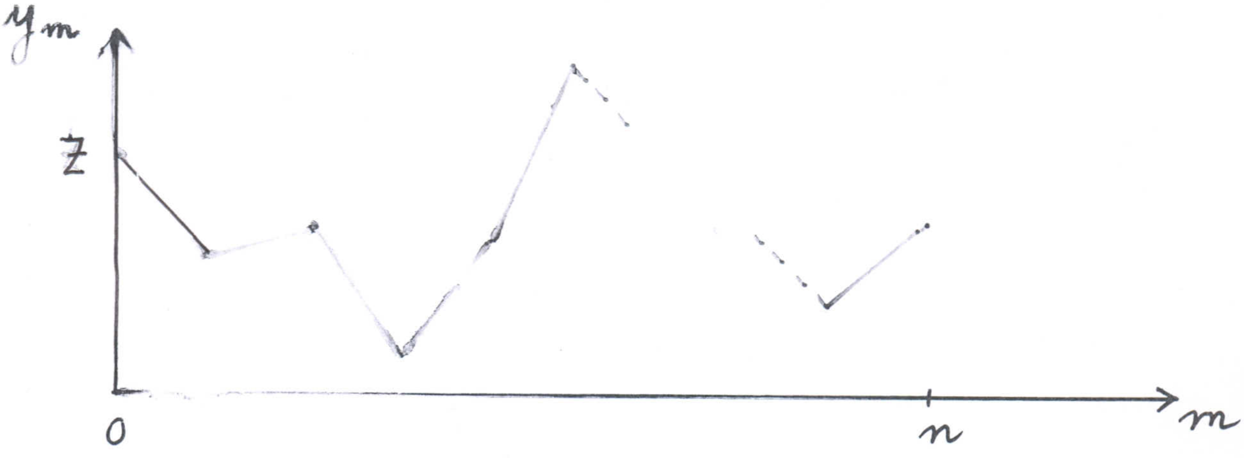
$f(y)$ continuous, symmetric

$$\sigma^2 = \int_{-\infty}^{+\infty} y^2 f(y)\, dy < \infty$$

- Maximum $\quad M_n = \max\,[0, x_1, x_2, \ldots x_n]$

$$Q_n(z) = \text{Prob}\,[M_n < z]$$

$$x_m \longrightarrow y_m = z - x_m$$



$$Q_n(z) = \mathrm{Prob}\,[M_n < z]$$

$$= \mathrm{Prob}\,[y_1 > 0, y_2 > 0, \dots y_n > 0 \mid y_0 = z]$$

. Recursion relation

$$Q_n(z) = \int_0^\infty Q_{n-1}(z')\, f(z - z')\, dz'$$

$$\begin{cases} Q_0(z) = 1 \\ z \geqslant 0 \end{cases}$$

. Generating function

$$\tilde{Q}(z,s) = \sum_{n=0}^{\infty} s^n Q_n(z)$$

Inhomogeneous Wiener - Hopf equation

$$\boxed{\tilde{Q}(z,s) = s \int_0^\infty f(z - z')\, \tilde{Q}(z',s)\, dz' + 1}$$

$$\sum_{n=0}^{\infty} s^n E\left(e^{-p M_n}\right) = p \int_0^\infty \tilde{Q}(z,s)\, e^{-pz}\, dz$$

· Solution : Pollaczek - Spitzer

$$\cdot \int_0^\infty \tilde{Q}(z,s)\, e^{-pz}\, dz = \frac{1}{p\sqrt{1-s}} \exp - \frac{p}{\pi} \int_0^\infty \frac{\ln(1 - s\,\hat{f}(k))}{p^2 + k^2}$$

$$\cdot \sum_{n=0}^{\infty} s^n\, E\left(e^{-p M_n}\right) = \frac{1}{\sqrt{1-s}} \exp - \frac{p}{\pi} \int_0^\infty \frac{\ln(1 - s\,\hat{f}(k}{p^2 + k^2}$$

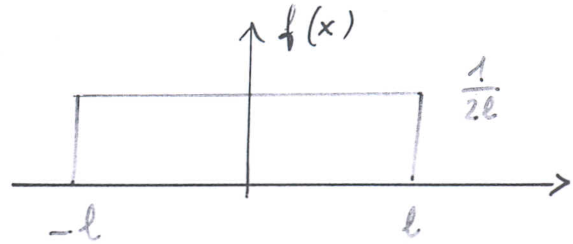
Extracting the singular part $s \to 1$, $p \to 0$ gives

$$\boxed{E(M_n) = \sigma \sqrt{\frac{2n}{\pi}} + \frac{1}{\pi} \int_0^\infty \frac{dk}{k^2} \log \frac{1 - \hat{f}(k)}{\sigma^2 k^2/2} + O\left(\frac{1}{\sqrt{n}}\right)}$$

where $\hat{f}(k) = \int_{-\infty}^{+\infty} f(x)\, e^{ikx}\, dx$ $\left\{ \begin{array}{l} \text{S.N. Majumd} \\ \text{A.C} \end{array} \right.$

Example

uniform jump distribution



$$\hat{f}(k) = \frac{\sin k\ell}{k\ell}$$

$$\sigma^2 = \ell^2/3$$

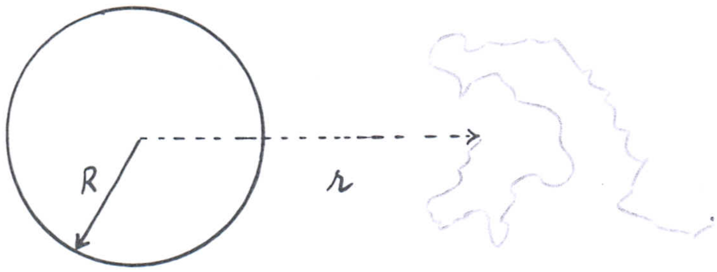
$$E(M_n) = \sigma \sqrt{\frac{2n}{\pi}} - C\ell + O\left(\frac{1}{\sqrt{n}}\right)$$

$$C = -\frac{1}{\pi} \int_0^\infty \frac{dk}{k^2} \log\left[\frac{6}{k^2}\left(1 - \frac{\sin k}{k}\right)\right] = 0{,}29795219 02$$

Problem II.

Capture of a particle to a spherical trap in 3 d

(Cf. Smolucho



- $P(\vec{r},t) =$ probability that a particle at initial posit $\vec{r}$ survives up to time t.

$$= \int d^3\vec{r}\,' \; G(\vec{r}\,', t' \,|\, \vec{r}\; 0)$$

- Backward diffusion equation

$$\frac{\partial P}{\partial t} = D \,\Delta P \qquad |\vec{r}| \geq R$$

$$\begin{cases} P(\vec{r}, 0) = 1 & |\vec{r}| > R \\ P(|\vec{r}| = R, t) = 0 & \forall t \end{cases}$$

- Spherical symmetry

$$\frac{\partial P}{\partial t} = D \left(\frac{\partial^2 P}{\partial r^2} + \frac{2}{r} \frac{\partial P}{\partial r} \right)$$

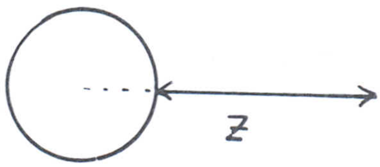
$$P(\vec{r}, t) = \frac{F(r,t)}{r}$$

$$\frac{\partial F}{\partial t} = D \frac{\partial^2 F}{\partial r^2} \qquad \begin{cases} F(r, 0) = r \\ F(R, t) = 0 & \forall t \end{cases}$$

$$r \geq R$$

Effective 1 d diffusion equation

$$z = r - R \geq 0$$



$$Q(z,t) \equiv F(r - R, t)$$

$$\frac{\partial Q}{\partial t} = D \frac{\partial^2 Q}{\partial z^2}$$

$$\begin{cases} Q(z,0) = R + z & \longrightarrow \text{initial condition} \\ Q(z=0,t) = 0 \quad \forall t & \longrightarrow \text{absorption} \end{cases}$$

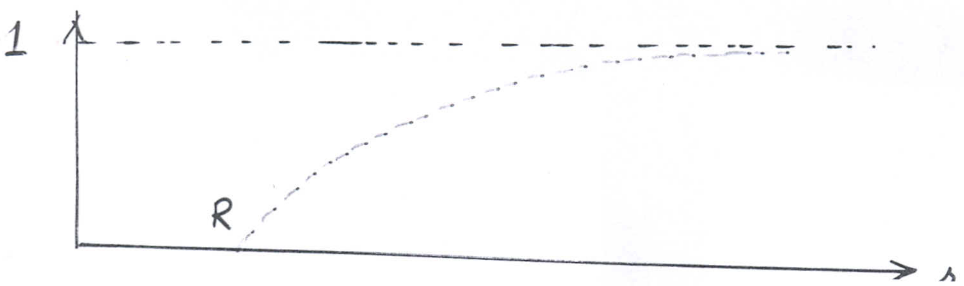
. Solution

$$Q(z,t) = z + \frac{2R}{\sqrt{\pi}} \int_0^{\frac{z}{\sqrt{4Dt}}} e^{-u^2} du$$

$$\boxed{P(r,t) = 1 - \frac{R}{r} \frac{2}{\sqrt{\pi}} \int_{\frac{r-R}{\sqrt{4Dt}}}^{\infty} e^{-u^2} du}$$

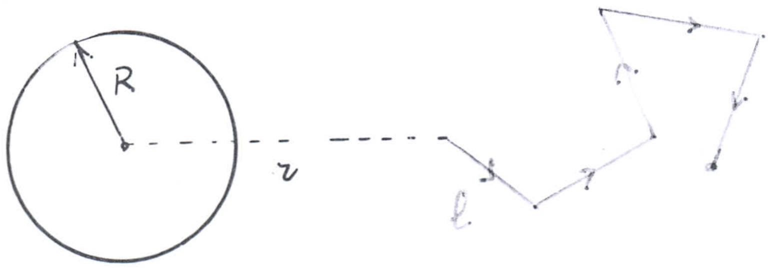
. Stationnary survival probability

$$\lim_{t \to \infty} P(r,t) = P(r,\infty) = 1 - \frac{R}{r}$$



Discrete random walk outside a trap

. Physical picture: the case of ~~Rayleigh~~ Pearson flights (Ziff, 9

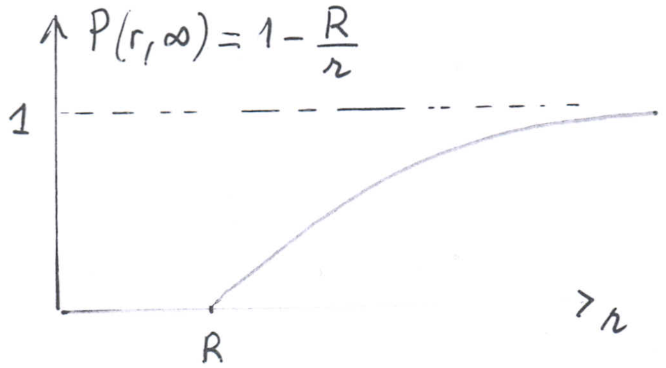


$$W(\vec{r},\vec{r}\,') = \frac{1}{4\pi}\,\delta\left(|\vec{r}-\vec{r}\,'| - \ell\right)$$

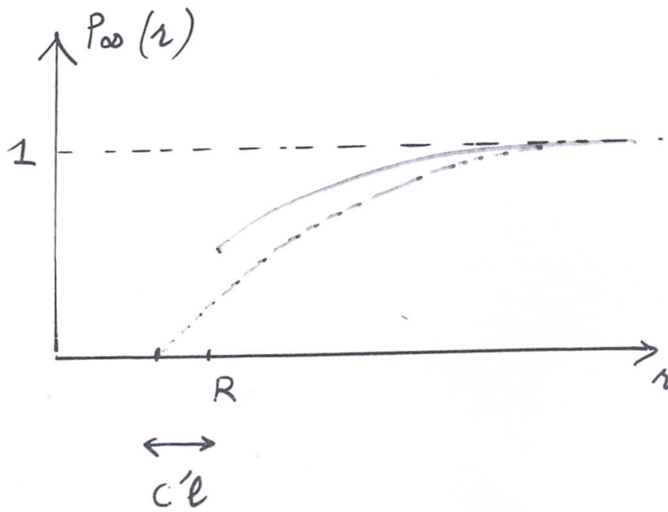
. Survival probability

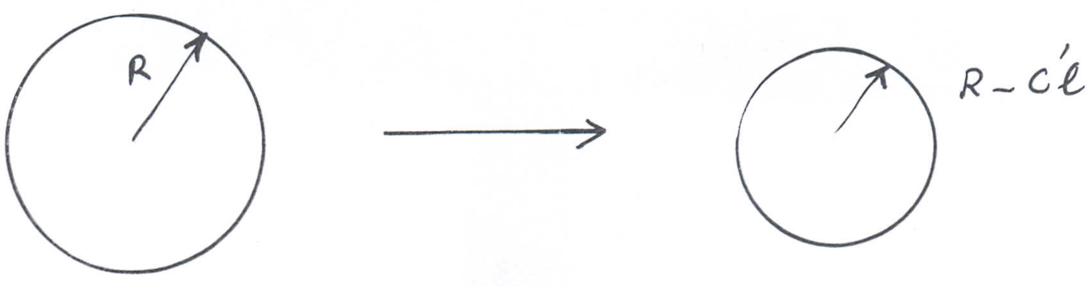
$$\lim_{n\to\infty} P_n(r) \begin{cases} \xrightarrow[r \geq R]{} 1 - \dfrac{R - C'\ell}{r} & C' = 0{,}29 \\[2ex] \xrightarrow[r \to R]{} 0{,}4082\,\dfrac{\ell}{R} \end{cases}$$

Brownian motion

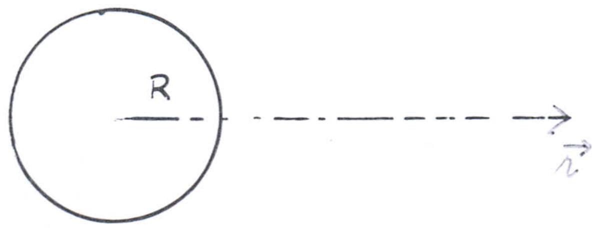


Random walk





Integral equation for an arbitrary isotropic jump distribution



$$P_n(\vec{r}) = \int P_{n-1}(\vec{r}\,')\, W(|\vec{r}-\vec{r}\,'|)\, d\vec{r}\,'$$

- Initial condition $\quad P_0(\vec{r}) = 1 \qquad |\vec{r}| > R$

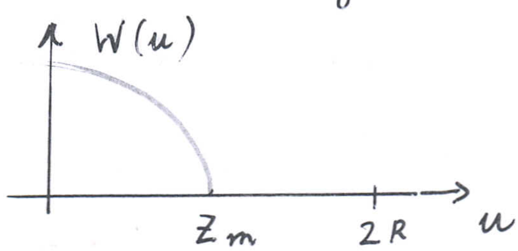
- Spherical symmetry

$$P_n(\vec{r}) = P_n(r)$$

$$P_n(r) = 2\pi \int_R^\infty dr'\, r'^2\, P_{n-1}(r') \int_0^\pi W\left(\sqrt{r^2+r'^2-2rr'\cos\theta}\right) \sin\theta\, d\theta$$

$$= \frac{2\pi}{r} \int_R^\infty dr'\, r'^2\, P_{n-1}(r') \int_{|r'-r|}^{r'+r} u\, W(u)\, du$$

- Bounded range



$$2\pi \int_{|r'-r|}^{r'+r} u\, W(u)\, du = f(|r'-r|)$$

$$\underbrace{r\, P_n(r)}_{F_n(r)} = \int_R^\infty r' \underbrace{P_{n-1}(r')}_{F_n(r')} f(|r'-r|)\, dr'$$

- Recursion relation

$$F_n(r) = \int_R^{\infty} F_{n-1}(r')\, f(|r'-r|)\, dr'$$

$$z = r - R \qquad Q_n(z) \equiv F_n(r - \cancel{R})$$

$$\begin{cases} Q_n(z) = \displaystyle\int_0^{\infty} Q_{n-1}(z')\, f(|z-z'|)\, dz' \\ Q_0(z) = R + z \end{cases}$$

- generating function

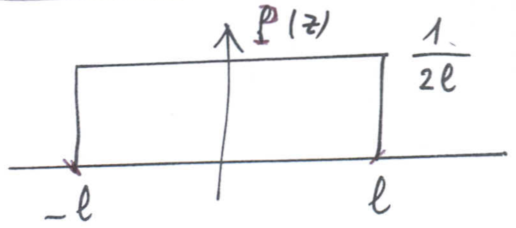
$$\tilde{Q}(z,s) = \sum_{n=0}^{\infty} s^n Q_n(z)$$

satisfies the inhomogeneous Wiener-Hopf equation

$$\boxed{\tilde{Q}(z,s) = s \int_0^{\infty} f(z-z')\, \tilde{Q}(z',s) + Q_0(z)}$$

3d $\longrightarrow$ 1d

$$W(|\vec{r}-\vec{r}'|) = \frac{1}{4\pi}\,\delta(|\vec{r}-\vec{r}'|-\ell)$$



$$Q_0(z) = z + R$$

different source term

Summary

- Problem I $\quad \tilde{Q}(z,s) = s \int_0^\infty f(z-z') \tilde{Q}(z',s)\, dz' +$

- Problem II $\quad \tilde{Q}(z,s) = s \int_0^\infty f(z-z') \tilde{Q}(z',s)\, dz' +$

- General inhomogeneous Wiener-Hopf problem

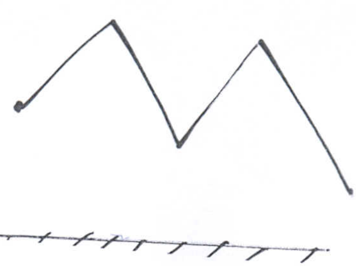
$$\tilde{Q}(z,s) = s \int_0^\infty f(z-z') \tilde{Q}(z',s) + \underset{\substack{\uparrow \\ \text{source}}}{J(z')}$$

- Half-space problems

  - radiative transfer in semi-infinite atmosphe

    - Wiener-Hopf
    - Chandrasekhar
    - Sobolev

$$S(\tau) = \underset{\substack{\downarrow \\ \text{probability absorption of photons}}}{\epsilon}\, B(\tau) + (1-\epsilon) \int_0^\infty K(\tau - t)\, S(t)\, dt$$



. General solution (Ivanov 1994)

$$\psi(z) = s \int_0^\infty f(z-z') \psi(z') \, dz' + J(z)$$

. Green's function

$$G(z, z_1) = s \int G(z', z_1) f(z-z') \, dz' + \delta(z-z_1)$$

Then

$$\psi(z) = \int_0^\infty G(z, z_1) J(z_1) \, dz_1$$

. Double Laplace transform

$$\tilde{G}(\lambda, \lambda_1) = \int_0^\infty dz \, e^{-\lambda z} \int_0^\infty dz_1 \, e^{-\lambda_1 z_1} \, G(z, z_1)$$

$$= \frac{\phi(\lambda)\,\phi(\lambda_1)}{\lambda + \lambda_1}$$

where

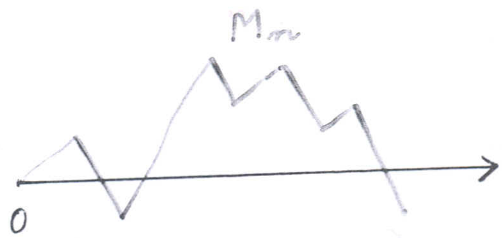
$$\phi(\lambda) = \exp - \frac{\lambda}{\pi} \int_0^\infty \frac{\log\left(1 - s \hat{f}(k)\right)}{\lambda^2 + k^2} \, dk$$

$$\hat{f}(k) = \int_{-\infty}^{+\infty} f(z) \, e^{ikz} \, dz$$

Results

Problem I : maximum of a 1 d random walk

$$Q_n(z) = \text{Prob}\,(M_n < z)$$

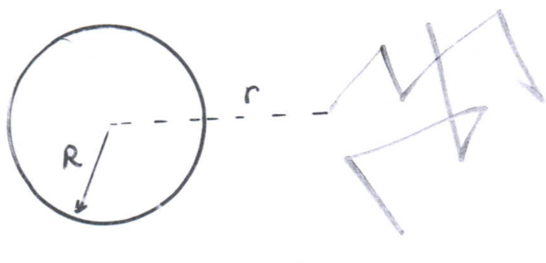


$$\sum_{n=0}^{\infty} s^n \int_0^{\infty} Q_n(z)\, e^{-pz}\, dz = \frac{1}{p\sqrt{1-s}} \exp - \frac{p}{\pi} \int_0^{\infty} \frac{dk \, \log\left(1 - s\hat{f}(k)\right)}{p^2 + k^2}$$

$$\Rightarrow \quad E(M_n) = \int_0^{\infty} z \frac{\partial Q_n}{\partial z} = \sigma \sqrt{\frac{2n}{\pi}} - A + O\left(\frac{1}{\sqrt{n}}\right)$$

$$\boxed{A = -\frac{1}{\pi} \int_0^{\infty} \frac{dk}{k^2} \log\left(\frac{1 - \hat{f}(k)}{\sigma^2 k^2/2}\right)}$$

Problem II asymptotic survival probability



$$P_\infty(r) = \frac{Q_\infty(z)}{r}$$

$$\int_0^{\infty} Q_\infty(z)\, e^{-pz}\, dz = \frac{1}{p^2} \exp - \frac{p}{\pi} \int_0^{\infty} \frac{dk}{k^2 + p^2} \log\left(\frac{1 - \cancel{s}\hat{f}(k)}{\sigma^2 k^2/2}\right)$$

$$\boxed{P(r) \xrightarrow{r \gg R} 1 - \frac{R - A}{r}} \qquad \boxed{P_\infty(R) = \frac{\sigma}{\sqrt{2}} \frac{1}{R}}$$

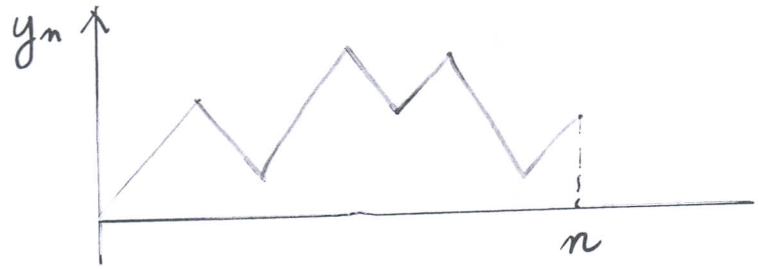
Probabilistic 3-d analogue of the Sparre-Andersen theorem

theorem: ξ_i iid random variables distributed with an even density $f(x)$

$$p_n = \text{Prob}\{\xi_1 > 0,\ \xi_1 + \xi_2 > 0, \ldots\ \xi_1 + \xi_2 + \cdots + \xi_n > 0\}$$

$$= \binom{2n}{n} 2^{-2n}$$ <u>independant</u> of $f(x)$

Note: $p_n = Q_n(0) =$ survival prob. up to step n

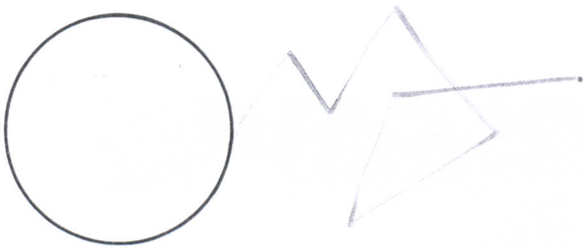


Solution of Wiener-Hopf equation

$$\Rightarrow \sum_{n=0}^{\infty} s^n Q_n(0) = \frac{1}{\sqrt{1-s}}$$

3 d analogue

$$P_\infty(R) = \frac{\sigma}{R\sqrt{2}}$$



$$\lim_{n \to \infty} \frac{R P_n(R)}{\sigma} = \frac{1}{\sqrt{2}}$$