Lecture notes on Stochastic processes

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INDEPENDENT & IDENTICALLY DISTRIBUTED (iid) RANDOM VARIABLES:

Consider: $\{x_1, x_2 \cdots x_N\}$

$$p(x_1, x_2, \cdots x_N) = \phi(x_1)\,\phi(x_2) \cdots \phi(x_N) \equiv \prod_{i=1}^{N} \phi(x_i).$$

In general:

$$\underbrace{p(x_1, x_2 \cdots x_N)} \neq \prod_{i=1}^{N} \phi(x_i)$$

The random variables are correlated.

$$\langle x_i x_j \rangle \neq \langle x_i \rangle \langle x_j \rangle$$

CHARACTERISTIC FUNCTION OF A RANDOM VARIABLE X:

$$\psi(k) = \langle e^{ikx} \rangle \equiv \int_{-\infty}^{+\infty} e^{ikx}\,\phi(x)\,dx.$$

Then:

$$\phi(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-ikx}\,\psi(k)\,dk.$$

Note: characteristic function is closely related to Fourier Tr.

- $\psi(0) = 1 \equiv \int_{-\infty}^{+\infty} \phi(x)\,dx$ (Normalization)
- Moments: $\langle x^n \rangle = (-i)^n \left.\dfrac{d^n \psi(k)}{dk^n}\right|_{k=0}$

CHARACTERISTIC FUNCTION OF GAUSSIAN RV:

$$\phi(x) = \frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$

Then:

$$\varphi(k) = \int_{-\infty}^{+\infty} e^{ikx}\,\phi(x)\,dx = e^{i\mu k - \sigma^2 k^2/2}$$

$$\equiv \langle e^{ikx} \rangle$$

(check).

SUM OF GAUSSIAN RANDOM VARIABLES:

$$y = \sum_{i=1}^{N} x_i \qquad \text{and} \quad \phi(x) = \frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-x^2/2\sigma^2}$$

$$\langle e^{iky} \rangle = \left\langle e^{ik\sum_{j=1}^{N} x_j} \right\rangle = \left\langle \prod_{j=1}^{N} e^{ikx_j} \right\rangle$$

$$= \prod_{j=1}^{N} \langle e^{ikx_j} \rangle \qquad \text{(iid)}.$$

$$= \prod_{j=1}^{N} e^{-\sigma^2 k^2/2}$$

$$= e^{-N\sigma^2 \frac{k^2}{2}} = e^{-\sigma_+^2 k^2/2}, \qquad \sigma_+ = \sqrt{N}\,\sigma$$

In fact: $\langle y^2 \rangle = \sum_{i=1}^{N} \langle x_i^2 \rangle = N\sigma^2$

Thus:

$$P(y) = \frac{1}{\sqrt{2\pi\sigma_+^2}}\, e^{-\frac{y^2}{2\sigma_+^2}} \qquad \sigma_+ = \sigma\sqrt{N}$$

- Sum of Gaussian RVs is again Gaussian.

Check: $\mu \neq 0$ case.

Note:

Let $\phi(X) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(X-\mu)^2}$

$\Rightarrow \quad X = \mu + \sigma x$

where, $p(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$

How do you show it?

- $p(x) = \phi(X = \mu + \sigma x) \cdot \left|\frac{dX}{dx}\right|$

- $\sum_{i=1}^{N} X_i = \mu N + \sigma \sum_{i=1}^{N} x_i$

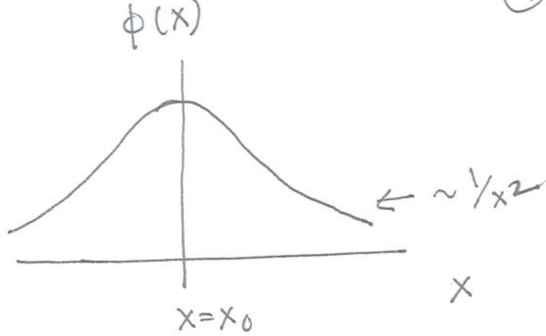
- $X = \mu + x$

$\Rightarrow \langle e^{ikX} \rangle = e^{i\mu k} \langle e^{ikx} \rangle$

What happens : $Y = \sum_{i=1}^{N} a_i X_i$?

CAUCHY DISTRIBUTION.

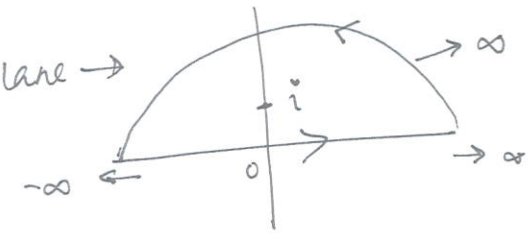
$$\phi(x) = \frac{1}{\pi} \frac{\gamma}{(x-x_0)^2 + \gamma^2}$$



Show:

(a) $\displaystyle\int_{-\infty}^{+\infty} \phi(x)\, dx = 1.$ (Normalization)

complex plane →



(b)

$$\varphi(k) = \langle e^{ikx} \rangle = \int_{-\infty}^{+\infty} e^{ikx} \phi(x)\, dx$$

For $k > 0$, close the contour through ~~the~~ the upper half:

For $k < 0$, " " " " lower half

$$\Rightarrow \boxed{\langle e^{ikx} \rangle = e^{ikx_0 - \gamma|k|}}$$

SUM: (Let $x_0 = 0$) $\quad y = \sum_{i=1}^{N} x_i$

$$\langle e^{iky} \rangle = \prod_{i=1}^{N} \langle e^{ikx_i} \rangle = e^{-\gamma N |k|} = e^{-\gamma_+ |k|}$$

$$\Rightarrow P(y) = \frac{1}{\pi} \frac{\gamma_+}{y^2 + \gamma_+^2}$$ is again CAUCHY. $\quad \gamma_+ = \gamma N$

LÉVY DISTRIBUTION

$$\phi(x) = \sqrt{\frac{c}{2\pi}} \; \frac{e^{-c/2x}}{x^{3/2}} \quad , \; x \geq 0$$

characteristic function:

$$\langle e^{ikx} \rangle = e^{-\sqrt{-2ick}} = e^{-|ck|^{1/2}(1-i\,\mathrm{sign}(k))}$$

[Will come back to it in the context of first-passage time]

Sum:

$$Y = \sum_{i=1}^{N} x_i$$

$$\langle e^{ikY} \rangle = \prod_{i=1}^{N} \langle e^{ikx_i} \rangle$$

$$= e^{-N\sqrt{-2ick}} = e^{-\sqrt{-2ic_+k}}$$

where $c_+ = N^2 c$

$$\Rightarrow \quad \phi(Y) = \sqrt{\frac{c_+}{2\pi}} \; \frac{e^{-c_+/2Y}}{Y^{3/2}} \quad \text{is again Lévy.}$$

Gaussian, Cauchy, Lévy are examples of stables distributions

STABLE DISTRIBUTION:

$$\langle e^{ikx} \rangle = \exp\left[i\mu k - |ck|^{\alpha} (1 - i\beta \,\mathrm{sgn}(k)\, \delta) \right]$$

where

$$\delta = \begin{cases} \tan\left(\frac{\pi\alpha}{2}\right) & \alpha \neq 1 \\ -\frac{2}{\pi} \log|k| & \alpha = 1 \end{cases}$$

$\alpha \in (0, 2]$

$\beta \in [-1, 1]$

SUM: $\quad Y = \sum_{i=1}^{N} x_i$

$$\langle e^{ikY} \rangle = \langle e^{ikx} \rangle^N = \exp\left[i\mu_+ k - |c_+ k|^{\alpha} (1 - i\beta \,\mathrm{sgn}(k)\, \delta) \right]$$

where, $\mu_+ = \mu N$

$c_+ = c N^{1/\alpha}$

Asymptotic behavior for $\alpha < 2$

$$\phi(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \langle e^{ikx} \rangle e^{-ikx} dk \sim \frac{A}{|x|^{1+\alpha}}$$

where

$$A = \alpha c^{\alpha} \left(1 + \beta \,\mathrm{sgn}(x)\right) \sin\left(\frac{\pi\alpha}{2}\right) \frac{\Gamma(\alpha)}{\pi}$$

- For $|\beta| = 1$, the support is on half-line.
- $\beta = 0 \rightarrow \phi(x)$ is symmetric about μ.

SPECIAL CASES OF STABLE DISTRIBUTION:

$(\mu = 0)$
$\mu \neq 0$ is a trivial shift

(1) $\alpha = 2$: $\Rightarrow \delta = 0$

$$\Rightarrow \langle e^{ikx} \rangle = e^{-|ck|^2}$$

$\Rightarrow \phi(x)$ is Gaussian with $\sigma^2 = 2c^2$

(2) $\alpha = 1, \beta = 0$:

$$\langle e^{ikx} \rangle = e^{-|ck|}$$

$\Rightarrow \phi(x)$ is CAUCHY.

(3) $\alpha = 1/2, \beta = 1$: $\Rightarrow \delta = 1$

$$\langle e^{ikx} \rangle = e^{-|ck|^{1/2}(1 - i\,\mathrm{sgn}(k))} = e^{-\sqrt{-2ick}}$$

$\Rightarrow \phi(x)$ is LÉVY.

SUM OF GAUSSIAN RANDOM VARIABLES: REVISITED.

For iid, we saw that the sum is again Gaussian.

What happens when the variables are correlated?

$$Y = \sum_{i=1}^{N} x_i$$

Let $\underline{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix}$ $\qquad \underline{\Sigma}_{N\times N} = \langle \underline{X}\, \underline{X}^T \rangle$

$$= \begin{bmatrix} \langle x_1^2 \rangle & \langle x_1 x_2 \rangle & \cdots & \langle x_1 x_N \rangle \\ \langle x_1 x_2 \rangle & \langle x_2^2 \rangle & \cdots & \\ \vdots & & \ddots & \\ \langle x_1 x_N \rangle & \cdots & \cdots & \langle x_N^2 \rangle \end{bmatrix}$$

$$\phi(\underline{x}) = \frac{1}{(2\pi)^{N/2} |\underline{\Sigma}|^{1/2}} e^{-\frac{1}{2} \underline{x}^T \underline{\Sigma}^{-1} \underline{x}}$$

$$\sum_{i=1}^{N} x_i = \underline{I}_1^T \underline{x} \qquad \text{where} \quad \underline{I}_1 = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}_{N\times 1}$$

$$\langle e^{ikY} \rangle = \left\langle e^{ik \sum_{j=1}^{N} x_j} \right\rangle$$

$$= \int_{-\infty}^{+\infty} d^N \underline{x} \; \frac{1}{(2\pi)^{N/2} |\underline{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2} \underline{x}^T \underline{\Sigma}^{-1} \underline{x} + ik \underline{I}_1^T \underline{x} \right)$$

$$= \exp\left(-\frac{k^2}{2} \underline{I}_1^T \underline{\Sigma}\, \underline{I}_1 \right)$$

$$\underline{I}_1^T \underline{\Sigma}\, \underline{I}_1 = \sum_{i,j}^{N} \underline{\Sigma}_{ij} \quad (\text{sum of elements of } \underline{\Sigma})$$

$$= \left\langle \left(\sum_{i=1}^{N} x_i \right)^2 \right\rangle = \langle y^2 \rangle = \sigma^2$$

$\cancel{\Rightarrow p(y) =}$

$$\Rightarrow \langle e^{iky} \rangle = e^{-\frac{k^2 \sigma^2}{2}}$$

$$\Rightarrow p(y) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{y^2}{2\sigma^2}} \quad \text{is Gaussian.}$$

- SUM OF GAUSSIAN RANDOM VARIABLES (either correlated or uncorrelated) is AGAIN GAUSSIAN.

STATE WITHOUT PROOF:

If $\underline{y(\tau) = \int_0^\tau \eta(t)\,dt}$, where $\eta(t)$ are Gaussian with mean $\underline{\langle \eta(t) \rangle = 0}$ and correlator $\underline{\langle \eta(t)\eta(t') \rangle = C(t,t')}$

then,

$$p(y) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{y^2}{2\sigma^2}} \quad \text{where } \sigma^2 = \langle y^2 \rangle.$$

CENTRAL LIMIT THEOREM:

$$Y = \sum_{i=1}^{N} x_i \qquad \left\{ \begin{array}{l} \langle x_i \rangle = 0 \\ \langle x_i^2 \rangle = \sigma^2 \\ \langle x_i x_j \rangle = 0 \text{ for } i \neq j \end{array} \right.$$

$\Rightarrow$

$$\langle Y \rangle = \sum_{i=1}^{N} \langle x_i \rangle = 0$$

$$\langle Y^2 \rangle = \left\langle \left(\sum_{i=1}^{N} x_i \right)^2 \right\rangle = \sum_{i=1}^{N} \langle x_i^2 \rangle = \sigma^2 N$$

$$\Rightarrow \sqrt{\langle Y^2 \rangle} = \sigma \sqrt{N}$$

- Let $Z = \dfrac{Y}{\sigma\sqrt{N}} \equiv \dfrac{\sum_{i=1}^{N} x_i}{\sigma\sqrt{N}} \Rightarrow \langle Z \rangle = 0$ & $\langle Z^2 \rangle = 1$

- $$\langle e^{ikZ} \rangle = \left\langle e^{ik \sum_{j=1}^{N} x_j / (\sigma\sqrt{N})} \right\rangle$$

$$= \left\langle \prod_{j=1}^{N} e^{ik \frac{x_j}{\sigma\sqrt{N}}} \right\rangle = \prod_{j=1}^{N} \left\langle e^{ik \frac{x_j}{\sigma\sqrt{N}}} \right\rangle$$

$$\Rightarrow \langle e^{ikZ} \rangle = \left\langle e^{ik \frac{x}{\sigma\sqrt{N}}} \right\rangle^N$$

Now, $\cancel{\langle x^2 \rangle}$

$$\langle x \rangle = -i \frac{d}{dk} \langle e^{ikx} \rangle \Big|_{k=0}$$

$$\langle x^2 \rangle = -\frac{d^2}{dk^2} \langle e^{ikx} \rangle \Big|_{k=0}$$

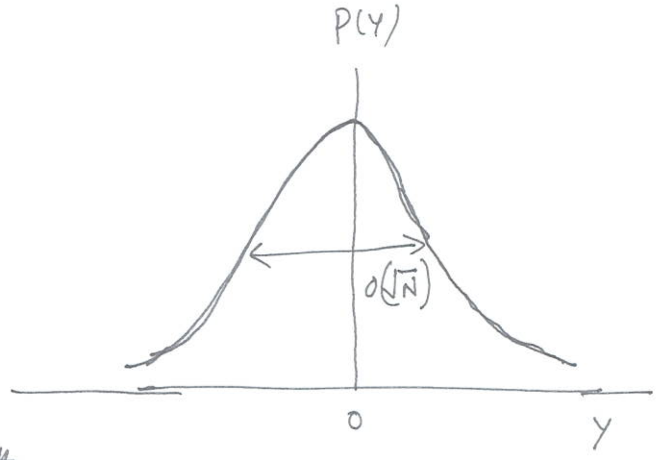
Since $\langle x \rangle = 0$ and $\langle x^2 \rangle = \sigma^2$ is finite

$$\Rightarrow \langle e^{ikx} \rangle = 1 - \frac{k^2\sigma^2}{2} + o(k^2)$$

$$\Rightarrow \left\langle e^{ik\frac{x}{\sigma\sqrt{N}}} \right\rangle = 1 - \frac{k^2}{2N} + o\left(\frac{k^2}{N}\right)$$

$$\Rightarrow \langle e^{ikz} \rangle = \left[1 - \frac{k^2}{2N} + o\left(\frac{k^2}{N}\right)\right]^N \xrightarrow{N\to\infty} e^{-k^2/2}$$

$$\Rightarrow \boxed{\lim_{N\to\infty} p(z) = \frac{1}{\sqrt{2\pi}} e^{-z^2/2}}$$ is Gaussian.



• $Y = \sum_{i=1}^{N} x_i = \sigma\sqrt{N}\, z$

$\cancel{\Rightarrow P(Y) = p(z)}$

$$\Rightarrow P(Y) = p\left(z = \frac{Y}{\sigma\sqrt{N}}\right)\left|\frac{dz}{dy}\right|$$

$$\Rightarrow P(Y) \approx \frac{1}{\sqrt{2\pi\sigma^2 N}} e^{-\frac{Y^2}{2\sigma^2 N}}$$ for large N.

and $0 \lesssim Y \lesssim O(\sqrt{N})$.

~~ie $Y \sim O(\sqrt{N})$.~~

What happens when $Y \gg O(\sqrt{N})$ ie $Y \sim O(N)$?
We will come back to it later in the context of RW.

LAW OF LARGE NUMBERS:

$$Y = \sum_{i=1}^{N} x_i$$

$$= N\mu + \sum_{i=1}^{N} \omega_i$$

$$\Rightarrow Y = N\mu + \sqrt{N}\, Z$$

where $p(z) = \frac{1}{\sqrt{2\pi}} e^{-z^2/2}$

$$\langle x_i \rangle = \mu$$

$$\left\langle \left[x_i - \langle x_i \rangle \right]^2 \right\rangle = 1$$

$$\parallel$$

$$\langle x_i^2 \rangle - \langle x_i \rangle^2$$

Let $x_i = \mu + \omega_i$

$$\Rightarrow \langle \omega_i \rangle = 0$$

$$\langle \omega_i^2 \rangle = 1$$

Now,

$$M = \frac{1}{N} \sum_{i=1}^{N} x_i = \frac{Y}{N} = \mu + \frac{1}{\sqrt{N}} z.$$

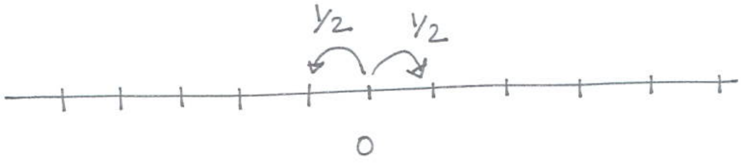
$$\text{or} \quad M \xrightarrow{N \to \infty} \mu.$$

SAMPLE AVERAGE CONVERGES TO THE EXPECTED VALUE FOR LARGE N.

THE ERROR DECREASES AS N INCREASES as $\frac{1}{\sqrt{N}}$

ie ERROR $\propto \frac{1}{\sqrt{N}}$ in simulations or experiments

RANDOM WALK: IN ONE-DIMENSION



$p+q=1$.

Home work:

- $x_n = x_{n-1} + \xi_n$ Let $x_0 = 0$

$$\xi_n = \begin{cases} 1 & \text{with prob } 1/2 \\ -1 & \text{" " "} \end{cases}$$

$P(x,N)$ = Prob that the walker is at position x at the end of Nth step.

i.e. $$p(\xi) = \begin{cases} 1/2 & \text{if } \xi = \pm 1 \\ 0 & \text{otherwise} \end{cases}$$

Possible values of x are*:

$-N, -N+1, -N+2, \cdots -1, 0, 1, \cdots +N-2, N-1, N.$

[* ONLY ODD/EVEN VALUES ARE POSSIBLE DEPENDING ON N ODD/EVEN]

Quick answer for large N:

$\langle \xi \rangle = 0$

$\langle \xi^2 \rangle = 1.$

$$x_1 = \xi_1$$

$$x_2 = x_1 + \xi_2 = \xi_1 + \xi_2$$

$$x_3 = x_2 + \xi_3 = \xi_1 + \xi_2 + \xi_3.$$

$$\vdots$$

$$x_N = \sum_{i=1}^{N} \xi_i$$ ← SUM OF RANDOM VARIABLES

$\Rightarrow \langle x_N \rangle = 0$ and $\langle x_N^2 \rangle = N$.

CENTRAL LIMIT THEOREM (BLINDLY) $\Rightarrow$

$$p^*(x,N) = \frac{1}{\sqrt{2\pi N}} e^{-\frac{x^2}{2N}}.$$

Prob that $x_N = x$.

However, ~~$P^*(X,N)$~~

X is EVEN (ODD) if N is EVEN (ODD).

THEREFORE, PROBABILITIES ~~EB~~ for X odd (even) $= 0$ and for even (odd):

$$\Rightarrow \quad P(X,N) = 2P^*(X,N) = \left(\frac{2}{\pi N}\right)^{1/2} e^{-X^2/2N}.$$

EXACT SOLUTION:

(1) $$P(x,n) = \frac{1}{2}\left[P(x+1,n) + P(x-1,n)\right]$$

Solve by using $\tilde{P}(k,n) = \sum_{x=-\infty}^{+\infty} P(x,n)\, e^{ikx}$

with $P(x,0) = \delta_{x,0}$

(2) $$\langle e^{ikx}\rangle = \left\langle e^{ik\sum_{j=1}^{N}\xi_j}\right\rangle = \langle e^{ik\xi}\rangle^N$$

$$\langle e^{ikx}\rangle = \sum_{x=-\infty}^{+\infty} e^{ikx} P(x,N)$$

$$\langle e^{ik\xi}\rangle^N = \left[\frac{1}{2}e^{ik} + \frac{1}{2}e^{-ik}\right]^N$$

$$= \frac{1}{2^N}\sum_{r=0}^{N}\binom{N}{r} e^{ikr} e^{-ik(N-r)}$$

$$= \frac{1}{2^N}\sum_{r=0}^{N}\binom{N}{r} e^{ik(2r-N)}$$

$$= \frac{1}{2^N}\sum_{x=-N}^{N}\binom{N}{\frac{N+x}{2}} e^{ikx}$$

$$\Rightarrow \boxed{P(x,N) = \frac{1}{2^N}\binom{N}{\frac{N+x}{2}}}$$

~~(3)~~ (3)

No. of left steps $= L$

No of right steps $= R$.

Total no. of steps $= L + R = N$

Final position $= X$ (say on right) $\Rightarrow$ $R - L = X$.

$$\Rightarrow \quad R = \frac{N+X}{2}.$$

No. of ways of choosing R right steps ~~of~~ out of total N steps $= \binom{N}{R} = \binom{N}{\frac{N+X}{2}}$ = Total no of paths that ends at X

Probability of each path $= \left(\frac{1}{2}\right)^L \cdot \left(\frac{1}{2}\right)^R = \frac{1}{2^N}$.

$$\Rightarrow \quad P(X,N) = \frac{1}{2^N}\binom{N}{\frac{N+X}{2}} = \frac{1}{2^N}\,\frac{N!}{\left(\frac{N+X}{2}\right)!\left(\frac{N-X}{2}\right)!}.$$

STIRLING'S APPROXIMATION

$$n! \sim \sqrt{2\pi}\; n^{n+\frac{1}{2}}\, e^{-n}$$

$$+ \quad X \ll N: \quad \longrightarrow \quad P(X,N) = \left(\frac{2}{\pi N}\right)^{1/2} e^{-X^2/2N}$$

~~ie.~~

$$0 \le |X| \lesssim O(\sqrt{N}).$$

LARGE DEVIATION:

STIRLING APPROXIMATION

$$\rightarrow \quad P(X,N) \approx \left(\frac{2}{\pi N}\right)^{1/2} e^{-\frac{N}{2}\left[\left(1+\frac{X}{N}+\frac{1}{N}\right)\ln\left(1+\frac{X}{N}\right) + \left(1-\frac{X}{N}+\frac{1}{N}\right)\ln\left(1-\frac{X}{N}\right)\right]}$$

~~Now N → ∞~~

Now $N \gg 1$, $\quad \frac{X}{N} = z$

$$P(X,N) \sim e^{-N\,\Phi\left(\frac{X}{N}\right)}.$$

where, $\Phi(z) = \frac{1}{2}\left[(1+z)\ln(1+z) + (1-z)\ln(1-z)\right].$

large deviation function.

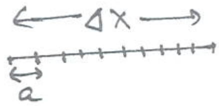
For $z \to 0$: $\quad \Phi(z) = -\frac{z^2}{2}.$

$$\Rightarrow P(X,N) \sim e^{-\frac{N}{2}\cdot\left(\frac{X}{N}\right)^2} = e^{-\frac{X^2}{2N}}.$$

COARSE-GRAINING:

Lattice spacing $= a$ $\qquad a \ll 1$.

$\Rightarrow$ Displacement $\cancel{\equiv}$ $y = x a$



Prob of the walker in the interval $(y, y+\Delta y)$ ~~when~~ ~~is~~ after N steps:

$[1 \gg \Delta y \gg a.]$

$$P(y,N)\,\Delta y = P\left(x = \frac{y}{a}\right)\frac{\Delta y}{2a}$$

[since x can take only odd or even values]

$$\Rightarrow \quad P(y,N) = \frac{1}{\sqrt{2\pi N a^2}}\, e^{-\frac{y^2}{2Na^2}}$$

Suppose there are n ~~dis~~ steps per unit time

Then the number of steps in $t = nt = N$.

$$\rightarrow \quad P(y,t) = \frac{1}{\sqrt{4\pi D t}}\, e^{-y^2/4Dt}$$

with $\underline{D = \frac{1}{2} n a^2}$

Suppose the ~~time~~ waiting time between two steps is Δt.

$\Rightarrow \Delta t \cdot n = 1$

$\Rightarrow n = 1/\Delta t$.

Continuum limit of random walk:

$$P(x, t+\Delta t) = \frac{1}{2}\left[P(x-a,t) + P(x+a,t)\right]$$

[a is lattice spacing.

$$= \frac{1}{2}\Big[P(x,t) - a\frac{\partial P}{\partial x} + \frac{a^2}{2}\frac{\partial^2 P}{\partial x^2} + \cdots$$

$$+ P(x,t) + a\frac{\partial P}{\partial x} + \frac{a^2}{2}\frac{\partial^2 P}{\partial x^2} + \cdots\Big]$$

$$\Rightarrow \frac{P(x,t+\Delta t) - P(x,t)}{\Delta t} = \frac{a^2}{2\Delta t}\frac{\partial^2 P}{\partial x^2} + \cdots$$

Lim $\Delta t \to 0$

$$\Rightarrow \boxed{\frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial x^2}} \quad \text{where } D = \lim_{\substack{a\to 0\\ \Delta t\to 0}} \frac{a^2}{2\Delta t}.$$

Diffusion equation.

RETURN PROBABILITY OF RANDOM WALK ON LATTICE:

R := Prob. that the random walk return to the origin, irrespective of the number of steps.

$P(\vec{x}, n)$:= Prob that the RW is at position $\vec{x}$ at n^{th} step, starting at $\vec{x}=0$. ~~step~~

$F(n)$:= First-passage probability to the origin. i.e. the prob. that the RW return to the origin for the first time at the n^{th} step.

(1) $$R = \sum_{n=1}^{\infty} F(n)$$

Return for the 1st time

Return ~~again~~ again in n-m steps (may also return in between)

(2) $$P(0,n) = \delta_{n,0} + \sum_{m=1}^{n} F(m)\, P(0, n-m)$$

(3) Let

$$f(z) = \sum_{n=0}^{\infty} P(0,n)\, z^n$$

$$g(z) = \sum_{n=1}^{\infty} F(n)\, z^n \longrightarrow g(1) = \sum_{n=1}^{\infty} F(n) = R$$

$\therefore$ (2) $\Rightarrow$ $$f(z) = 1 + g(z) f(z).$$

$$\Rightarrow \boxed{g(z) = 1 - \frac{1}{f(z)}.} \Rightarrow R = g(1) = 1 - \frac{1}{f(1)}$$

Random walk in d-dimension:

$$\vec{r}_n = \vec{r}_{n-1} + \vec{\xi}_n \qquad \text{where} \quad \vec{\xi}_n = \hat{e}_i \text{ with prob } \frac{1}{2d}.$$

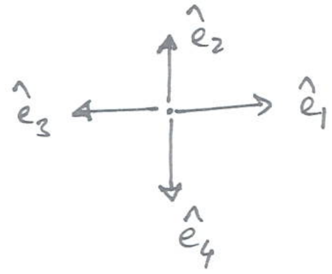
$i = 1, \cdots 2d.$

$$(3) \quad P(\vec{r}, n) = \frac{1}{2d} \sum_{i=1}^{2d} P(\vec{r} - \hat{e}_i, n-1)$$

for $n \geq 1$.

and $P(\vec{r}, 0) = \delta_{\vec{r}, 0}$

e.g. in 2d.



Define,

$$\tilde{P}(\vec{k}, n) = \sum_{\vec{r}} P(\vec{r}, n)\, e^{i\vec{k}\cdot\vec{r}}, \quad \vec{k} = (k_1, k_2 \cdots k_d)$$

then

$$P(\vec{r}, n) = \frac{1}{(2\pi)^d} \underbrace{\int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi}}_{d} d^d\vec{k}\; \tilde{P}(\vec{k}, n)\, e^{-i\vec{k}\cdot\vec{r}}$$

$$\Rightarrow \quad P(0, n) = \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \frac{d^d\vec{k}}{(2\pi)^d}\, \tilde{P}(\vec{k}, n).$$

$$(3) \Rightarrow \quad \tilde{P}(\vec{k}, n) = \left[\frac{1}{d} \sum_{i=1}^{d} \cos k_i\right] \tilde{P}(\vec{k}, n-1)$$

$$P(\vec{k}, 0) = 1. \quad \Rightarrow \quad \tilde{P}(\vec{k}, n) = \left[\frac{1}{d} \sum_{i=1}^{d} \cos k_i\right]^n$$

$$P(0,n) = \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \frac{d^d k}{(2\pi)^d} \left[\frac{1}{d} \sum_{i=1}^{d} \cos k_i \right]^n$$

$$\Rightarrow f(1) = \sum_{n=0}^{\infty} P(0,n)$$

$$= \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \frac{d^d \vec{k}}{(2\pi)^d} \frac{1}{1 - \frac{1}{d} \sum_{i=1}^{d} \cos k_i}$$

$$= \frac{d}{(2\pi)^d} \underbrace{\int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi}}_{d} \frac{d^d \vec{k}}{d - \sum_{i=1}^{d} \cos k_i}$$

~~Beh~~ Behavior of the integrand near $k=0$:

- $d - \sum_{i=1}^{d} \cos k_i = \frac{k^2}{2} + O(k^4)$

- $d^d \vec{k} \sim k^{d-1}\, dk$

~~$\Rightarrow$ Integrand $\sim$ k~~

$\Rightarrow$ Integral near $k=0 \sim \int k^{d-3} dk$.

$$R = \begin{cases} 0.340\ldots & \text{in } d=3 \\ 0.193\ldots & d=4 \\ 0.135\ldots & d=5 \\ 0.104\ldots & d=6 \\ 0.085\ldots & d=7 \\ 0.07\ldots & d=8 \end{cases}$$

For $d = 1$ & 2 : the integral diverges $\Rightarrow f(1) = \infty$

For $d \geq 3$: the integral is finite.

$$\rightarrow \quad R = \begin{cases} 1 & \text{for } d = 1 \,\&\, 2. \quad \text{(RW always come back)} \\ <1 & \text{for } d \geq 3. \quad \text{(Escapes to } \infty \text{ with finite prob)} \end{cases}$$

FIRST PASSAGE TIME PROBABILITY IN 1D.

$$g(z) = \sum_{n=1}^{\infty} F(n) z^n = 1 - \frac{1}{f(z)}$$

$$f(z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{dk}{1 - z\cos k} = \frac{1}{2\pi} \sum_{n=0}^{\infty} z^n \int_{-\pi}^{\pi} \cos^n k \, dk.$$

$$\int_{-\pi}^{\pi} \cos^n k \, dk = \int_{-\pi}^{\pi} \left(\frac{e^{ik} + e^{-ik}}{2}\right)^n = \sum_{r=0}^{n} \binom{n}{r} \frac{1}{2^n} \underbrace{\int_{-\pi}^{\pi} e^{ikm} \, dk}_{\text{where } m = 2r-n}$$

$$\begin{cases} = 0 & \text{for } m \neq 0 \\ = 2\pi & \text{for } m = 0 \Rightarrow r = n/2 \end{cases}$$

$$\Rightarrow \frac{1}{2\pi} \int_{-\pi}^{\pi} \cos^n k \, dk = \begin{cases} 0 & \text{for odd } n. \\ \binom{n}{n/2} \frac{1}{2^n} & \text{for even } n. \end{cases}$$

$$\Rightarrow f(z) = \sum_{n=0}^{\infty} \binom{2n}{n} \frac{z^{2n}}{2^{2n}} = \frac{1}{\sqrt{1-z^2}}$$

$$\Rightarrow \sum_{n=1}^{\infty} F(n) z^n = 1 - \sqrt{1-z^2} = \sum_{n=1}^{\infty} \binom{2n-2}{n-1} \frac{z^{2n}}{2^{2n-1}} \cdot \frac{1}{n}.$$

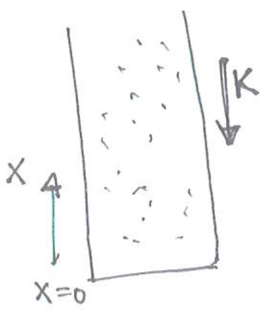
$$\Rightarrow F(2n+1) = 0 \qquad n = 0, 1, 2 \ldots$$

and $\boxed{F(2n) = \frac{1}{n} \binom{2n-2}{n-1} \frac{1}{2^{2n-1}}}$ $\quad n = 1, 2 \ldots$

$F(2n) \sim \frac{1}{n^{3/2}}$ for large n.

Einstein's fluctuation-dissipation relation (1905)

Imagine a dilute gas of noninteracting Brownian particles in a solvent under a constant force K (such as gravity) acts on each particle.



Osmotic pressure: $p(x) = \frac{RT}{N_A} \cdot \varrho(x)$

Force/volume due to the pressure field: $= -\frac{\partial p(x)}{\partial x}$. $\uparrow$ $\lim_{\Delta x \to 0} \frac{1}{\Delta x}\left[P(x) - P(x+\Delta x)\right]$

$P(x+\Delta x)$, $P(x)$, Δx

External force/volume: $= K\varrho(x)$. $\downarrow$

At equilibrium: (force balance)

(A) $$-\frac{RT}{N_A} \cdot \frac{\partial \varrho(x)}{\partial x} \pm K\varrho(x) \cancel{=0}.$$

Terminal velocity: $V = \frac{K}{6\pi\eta a}$.

Current due to external force $= \varrho(x) V$. $\downarrow$

Diffusion current: $= -D\frac{\partial \varrho(x)}{\partial x}$. $\uparrow$

$\frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial x^2}$

and $\frac{\partial \rho}{\partial t} + \nabla \cdot J_{drift} = 0$

At equilibrium: (current balance)

(B) $$-D\frac{\partial \varrho(x)}{\partial x} \pm \frac{K}{6\pi\eta a}\varrho(x) \cancel{=0}.$$

From (A) & (B) : $\boxed{D = \frac{RT}{N_A} \cdot \frac{1}{6\pi\eta a}}$ $= \frac{k_B T}{\gamma}$, $k_B = R/N_A$, $\gamma = 6\pi\eta a$

$\rho(x) = \rho(0)\, e^{-Kx/k_BT}$, $k_B = R/N_A$.
Boltzmann distribution.

Diffusion constant in terms of microscopic fluctuations:

D is defined as the proportionality constant between the diffusion current and the density gradient, i.e.

$$\boxed{J_{diff} = -D \frac{\partial \rho}{\partial t}}$$

For independent Brownian particles:

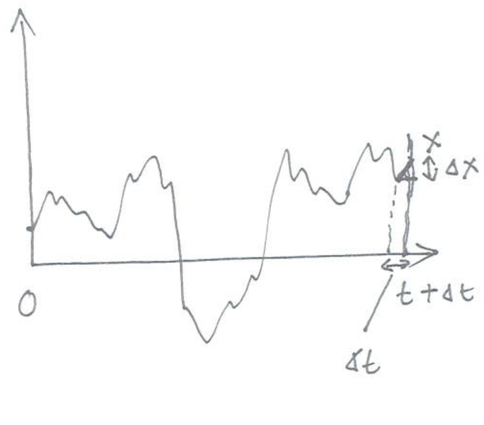
density $\equiv$ Probability density

i.e. $\rho(x,t) \equiv P(x,t)$.

where

$P(x,t)\,dx$ = Prob. that a particle is in ~~the~~ between x and $x+dx$ at time t.

$$(*) \quad P(x, t+\Delta t) = \int_{-\infty}^{+\infty} P(x-\Delta x, t)\, \phi_{\Delta t}(\Delta x)\, d(\Delta x)$$



where $\phi_{\Delta t}(\Delta x)$ is the normalized probability density of the jump Δx in time Δt.

$$\int_{-\infty}^{+\infty} \phi_{\Delta t}(\Delta x)\, d(\Delta x) = 1.$$

also, $\phi_{\Delta t}(\Delta x) = \phi_{\Delta t}(-\Delta x)$.

$$P(x-\Delta x, t) = P(x,t) - \Delta x \frac{\partial P}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 P}{\partial x^2} + \cdots$$

$$(*) \Rightarrow \quad P(x,t) + \Delta t \frac{\partial P}{\partial t} + \cdots = P(x,t) \underbrace{\int_{-\infty}^{+\infty} \phi_{\Delta t}(\Delta x)\, d(\Delta x)}_{=1}$$

$$- \frac{\partial P}{\partial x} \underbrace{\int_{-\infty}^{+\infty} \Delta x\, \phi_{\Delta t}(\Delta x)\, d(\Delta x)}_{=0}$$

$$+ \frac{\partial^2 P}{\partial x^2} \int_{-\infty}^{+\infty} \frac{(\Delta x)^2}{2} \phi_{\Delta t}(\Delta x)\, d(\Delta x)$$

$$+ \cdots$$

Putting

$$\frac{1}{\Delta t} \int_{-\infty}^{+\infty} \frac{(\Delta x)^2}{2} \phi_{\Delta t}(\Delta x)\, d(\Delta x) = D$$

then

$$\boxed{\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2}}$$ ← diffusion equation.

⇒ Coefficient of diffusion is related to the microscopic fluctuation; i.e.

$$\boxed{\langle (\Delta x)^2 \rangle = 2D\Delta t.}$$ or, $$\boxed{\lim_{\Delta t \to 0} \frac{\langle (\Delta x)^2 \rangle}{2\Delta t} = D.}$$

LANGEVIN DESCRIPTION OF BROWNIAN MOTION:

Local slope at time t:

$$\frac{\Delta x}{\Delta t} = \xi_{\Delta t}(t)$$

RANDOM 'NOISE' INDEPENDENT FROM ONE MICROSCOPIC STEP TO ANOTHER.

$$\langle \xi^2_{\Delta t}(t) \rangle = \frac{\langle (\Delta x)^2 \rangle}{(\Delta t)^2} = \frac{2D}{\Delta t} \quad \text{as } \Delta t \to 0.$$

$\Rightarrow$ $\xi_{\Delta t}(t)$ scales as $1/\sqrt{\Delta t}$ as $\Delta t \to 0$.

Since $\langle \Delta x \rangle = 0$

$$\langle \xi_{\Delta t}(t)\, \xi_{\Delta t}(t') \rangle = \begin{cases} 0 & \text{if } t \neq t' \\ \dfrac{2D}{\Delta t} & \text{if } t = t' \end{cases}$$

$$\sum_{\substack{t' \text{ in} \\ \text{steps of } \Delta t}} \langle \xi_{\Delta t}(t)\, \xi_{\Delta t}(t') \rangle = \frac{2D}{\Delta t} \cdot \Delta t = 2D.$$

$\Rightarrow$ In the limit $\Delta t \to 0$

$$\boxed{\frac{dx}{dt} = \xi(t)}$$

where $\langle \xi(t) \rangle = 0$

$\langle \xi(t)\, \xi(t') \rangle = 2D\, \delta(t-t')$.

LANGEVIN EQUATION (OVERDAMPED).

$\left[\; \dfrac{1}{\Delta t} \to \delta(0) \text{ as } \Delta t \to 0 \right.$

SOLUTION OF DIFFUSION EQUATION:

$$(*) \qquad \frac{\partial P(x,t)}{\partial t} = D\,\frac{\partial^2 P(x,t)}{\partial x^2}, \quad \text{and} \quad \begin{cases} P(x,0) = \delta(x - x_0). \\ P(x \to \pm\infty, t) = 0 \\ \left.\dfrac{\partial P}{\partial x}\right|_{x \to \pm\infty} = 0. \end{cases}$$

Define

$$\psi(k,t) = \int_{-\infty}^{+\infty} e^{ikx} P(x,t)\,dx \equiv \langle e^{ikx} \rangle$$

Then,

$$P(x,t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-ikx}\,\psi(k,t)\,dk.$$

$$\rightarrow \quad \int_{-\infty}^{+\infty} dx\,\frac{\partial P(x,t)}{\partial t}\,e^{ikx} = \frac{\partial}{\partial t}\int_{-\infty}^{+\infty} dx\,P(x,t)\,e^{ikx} = \frac{\partial \psi}{\partial t}.$$

$$\text{and,} \quad \int_{-\infty}^{+\infty} dx\,\frac{\partial^2 P}{\partial x^2}\,e^{ikx} = -k^2\,\psi(k,t).$$

[integrating by parts and using the B.C.]

$$(*) \Rightarrow \quad \frac{\partial \psi}{\partial t} = -k^2 D\,\psi \quad \Rightarrow \quad \psi(k,t) = \psi(k,0)\,e^{-k^2 D t}$$

$$\psi(k,0) = \int_{-\infty}^{+\infty} e^{ikx}\,\delta(x - x_0)\,dx = e^{ikx_0}.$$

$$\Rightarrow \quad \psi(k,t) = e^{ix_0 k - 2Dt k^2/2} \qquad (\sigma^2 = 2Dt)$$

$$\Rightarrow \quad \boxed{P(x,t) = \frac{1}{\sqrt{4\pi D t}}\,e^{-\frac{(x - x_0)^2}{4Dt}}}$$

For general $P(x,0)$:

$$\psi(k,0) = \int_{-\infty}^{+\infty} e^{ikx'} P(x',0)\, dx'$$

$$\Rightarrow \psi(k,t) = \int_{-\infty}^{+\infty} dx'\, P(x',0)\, e^{ikx' - 2Dt\frac{k^2}{2}}.$$

$$\Rightarrow P(x,t) = \int_{-\infty}^{+\infty} dx'\, P(x',0)\; G(x,t \mid x',0)$$

where

$$G(x,t \mid x',0) = \frac{1}{\sqrt{4\pi D t}}\, e^{-\frac{(x-x')^2}{4Dt}}$$

is the diffusion propagator, which denotes the conditional probability density that the Brownian particle reaches x at time t, starting from x_0 at $t=0$.

What about general d-dimensions:

(1) Show that in three dimensions $P(\vec{r},t)$ satisfies the differential equation: [Hint: the jumps in the three directions are independent.]

$$\frac{\partial P(\vec{r},t)}{\partial t} = D\nabla^2 P(\vec{r},t). \qquad \text{where } \vec{r} = (x,y,z)$$

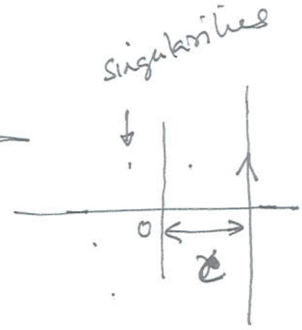
(2) Show that the ~~st~~ propagator corresponding to the above equation is: [Hint: Use higher dimensional F.T.]

$$G(\vec{r},t \mid \vec{r}_0,0) = \frac{1}{(4\pi D t)^{3/2}}\, e^{-\frac{(\vec{r}-\vec{r}_0)^2}{4Dt}}.$$

Solution of 1D diffusion by Laplace transform method:

LAPLACE TRANSFORM:

$$\left[\begin{array}{l} F(s) = \mathcal{L}\{f(t)\} = \int_0^\infty e^{-st} f(t)\, dt . \\ f(t) = \mathcal{L}^{-1}\{F(s)\} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{st} F(s)\, ds . \end{array}\right]$$



BROMWICH INTEGRAL

* Example

Useful property:

Suppose $g(t) = e^{-at} f(t)$

$$\mathcal{L}\{g(t)\} = \int_0^\infty e^{-st} e^{-at} f(t)\, dt = F(s+a) .$$

where

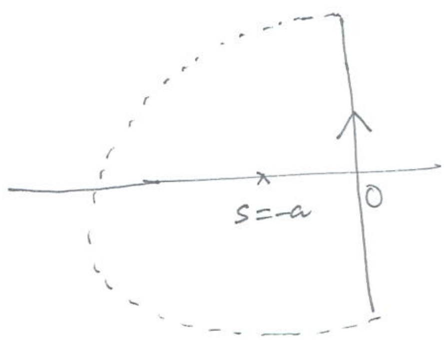
$$F(s) = \mathcal{L}\{f(t)\}$$

$\Rightarrow \cancel{F(s+a)}$

$$\Rightarrow \mathcal{L}^{-1}\{F(s+a)\} = g(t) = e^{-at} f(t) = e^{-at} \mathcal{L}^{-1}\{F(s)\} .$$

* $f(t) = e^{-at}$.

$$F(s) = \int_0^\infty e^{-st} e^{-at} = \frac{1}{s+a}$$



Now, $f(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{st} \frac{1}{s+a}\, ds .$

$c = 0$

[Residue thm] $= \frac{1}{2\pi i} \cdot 2\pi i \; e^{-at} = e^{-at}$

- 1D diffusion equation:

$$* \quad \boxed{\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^2 P(x,t)}{\partial x^2}}, \qquad \text{Boundary condition. } P(x\to\pm\infty,t)=0.$$

- Let us define the Laplace transform:

$$\Psi(x,s) = \int_0^\infty e^{-st}P(x,t)\,dt \qquad \Big|\ \Psi(x\to\pm\infty,s)=0$$

Then,

$$\int_0^\infty e^{-st}\frac{\partial P}{\partial t}\,dt = e^{-st}P(x,t)\Big|_0^\infty + s\int_0^\infty e^{-st}P(x,t)\,dt.$$

$$= -P(x,0) + s\Psi(x,s).$$

$$* \Rightarrow \boxed{D\frac{d^2\Psi}{dx^2} - s\Psi = -P(x,0).} \quad \leftarrow \text{INHOMOGENEOUS}$$

GREEN'S FUNCTION METHOD:

$$\Psi(x,s) = \int_{-\infty}^{+\infty} P(x',0)\,g(x,x';s)\,dx'$$

where $g(x,x';s)$ is the Green's function, which satisfies

$$\left[D\frac{d^2}{dx^2} - s\right]g(x,x';s) = -\delta(x-x').$$

$L_x\Psi(x) = f(x) \rightarrow \Psi(x) = \int f(x')\,g(x,x')\,dx'$, with $L_x g(x,x') = \delta(x-x')$

$L_x\Psi(x) = \int dx' f(x')\,L_x g(x,x') = \int dx' f(x')\,\delta(x-x') = f(x)$

Now, if $$\psi(x,s) = \int_{-\infty}^{+\infty} P(x',0)\, g(x,x';s)\, dx'$$

then,

$$P(x,t) = \mathcal{L}_s^{-1}\{\psi(x,s)\} = \int_{-\infty}^{+\infty} dx'\, P(x',0) . \mathcal{L}_s^{-1}\{g(x,x';s)\}.$$

$$\Rightarrow \quad P(x,t) = \int_{-\infty}^{+\infty} P(x',0)\, G(x,t\,|\,x',0)\, dx'$$

with, $$\underline{\underline{G(x,t\,|\,x',0)}} = \mathcal{L}_s^{-1}\{g(x,x';s)\}.$$

PROPAGATOR.

$$\star \quad \left[D\frac{d^2}{dx^2} - s\right] g(x,x';s) = -\delta(x-x').$$

(1) $x > x'$: $\left[D\frac{d^2}{dx^2} - s\right] g_>(x,x';s) = 0, \quad g_>(\infty,x';s) = 0$

(2) $x < x'$: $\left[D\frac{d^2}{dx^2} - s\right] g_<(x,x';s) = 0, \quad g_<(-\infty,x';s) = 0$

(3) At $x = x'$

Integrating $\star$ around x'

(a) $g_>(x',x';s) = g_<(x',x';s)$.

(b) $$D\left[\frac{d}{dx} g_>(x,x';s)\Big|_{x=x'} - \frac{d}{dx} g_<(x,x';s)\Big|_{x=x'}\right] = -1.$$

$$(1) \Rightarrow \quad g_{>}(x, x'; s) = A\, e^{-\sqrt{s/D}\, x}$$

$$(2) \Rightarrow \quad g_{<}(x, x'; s) = B\, e^{\sqrt{s/D}\, x}$$

$$(3.a) \Rightarrow \quad \cancel{A = B e^{2\sqrt{s/D}\, x'}} \quad A\, e^{-\sqrt{s/D}\, x'} = B\, e^{\sqrt{s/D}\, x'} .$$

$$(3.b) \Rightarrow \quad \sqrt{sD} \left[A\, e^{-\sqrt{s/D}\, x'} + B\, e^{\sqrt{s/D}\, x'} \right] = 1 .$$

$$B = \frac{1}{2\sqrt{sD}}\, e^{-\sqrt{s/D}\, x'}$$

$$A = \frac{1}{2\sqrt{sD}}\, e^{\sqrt{s/D}\, x'} .$$

$$\Rightarrow \begin{cases} g_{>}(x, x'; s) = \dfrac{1}{2\sqrt{sD}}\, e^{-\sqrt{s/D}\,(x - x')} \\ g_{<}(x, x'; s) = \dfrac{1}{2\sqrt{sD}}\, e^{-\sqrt{s/D}\,(x' - x')} . \end{cases}$$

$$\boxed{g(x, x'; s) = \frac{1}{\sqrt{4D}} \cdot \frac{e^{-\frac{|x - x'|}{\sqrt{D}}\sqrt{s}}}{\sqrt{s}}} .$$

$$\Rightarrow \boxed{G(x, t \mid x', 0) = \frac{1}{\sqrt{4\pi D t}}\, e^{-\frac{(x - x')^2}{4Dt}}}$$

using:

$$\mathcal{L}_s^{-1}\left\{ \frac{e^{-a\sqrt{s}}}{\sqrt{s}} \right\} = \frac{e^{-a^2/4t}}{\sqrt{\pi t}}$$

DIFFUSION EQUATION $\longleftrightarrow$ SCHRÖDINGER EQUATION

$$\frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial x^2} \quad \Big| \quad i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}$$

$$P(x,t) \longleftrightarrow \psi(x,t).$$

$$D \longleftrightarrow \frac{\hbar^2}{2m}$$

$$t \longleftrightarrow \frac{i}{\hbar}t \qquad \text{(Wick rotation)}$$

* COME BACK TO THE CASE WITH EXTERNAL POTENTIAL.

PATH INTEGRALS IN QUANTUM MECHANICS:

- SCHRÖDINGER EQUATION

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi \quad ; \quad H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x).$$

- $$\psi(x,t) = \int_{-\infty}^{+\infty} \psi(x_0,0)\, G(x,t|x_0,0)\, dx_0$$

- $G(x,t|x_0,0) = \langle x|\, e^{-\frac{i}{\hbar}Ht}\, |x_0\rangle$ is the QM propagator

which satisfies:

$$\left(H - i\hbar\frac{\partial}{\partial t}\right) G(x,t|x_0,0) = -i\hbar\,\delta(x-x_0)\,\delta(t)$$

[REMEMBER A SIMILAR EQ. IN THE CONTEXT OF DIFFUSION]

- $$G(x,t|x_0,0) = \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}[x(\tau)] \exp\left[\frac{i}{\hbar}\int_0^t \underbrace{L(\dot{x},x,\tau)}_{\text{Lagrangian}}\, d\tau\right]$$

- FOR FREE PARTICLE: $L = \frac{1}{2}m\left(\frac{dx}{d\tau}\right)^2$

BROWNIAN MOTION AND PATH INTEGRALS:

$$\frac{dx}{dt} = \eta(t).$$

$$\langle \eta(t) \rangle = 0$$

$$\langle \eta(t)\eta(t') \rangle = 2D\,\delta(t-t').$$

- η arises from the collisions by the molecules (many) in the medium.

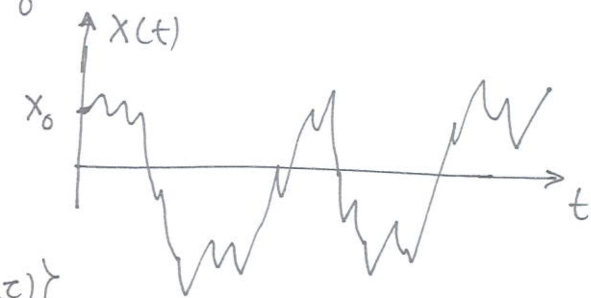
$$\eta = \sum(\text{RANDOM FORCES}).$$

CENTRAL LIMIT THEOREM $\longrightarrow$ η is GAUSSIAN.

- JOINT PROBABILITY DISTRIBUTION FOR A PARTICULAR NOISE REALIZATION $[\eta(\tau) : 0 \le \tau \le t]$

$$P[\{\eta(\tau)\}] \propto \exp\left[-\frac{1}{4D}\int_0^t \eta^2(\tau)\,d\tau\right]$$

$$\{\eta(\tau)\} \longrightarrow \{x(\tau)\}$$



- PROB. OF ANY PATH $\{x(\tau)\}$

$$P[\{x(\tau)\}] \propto 1.\left[-\frac{1}{4D}\int_0^t \left(\frac{dx}{d\tau}\right)^2 d\tau\right]$$

JACOBIAN OF TRANSFORMATION FROM $\{\eta(\tau)\}$ to $\{x(\tau)\}$.

- Diffusion propagator, i.e. the probability that a path goes from x_0 at $\tau=0$ to x at $\tau=t$.

$$G(x,t\,|\,x_0,0) = \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}[x(\tau)] \exp\left[-\frac{1}{4D}\int_0^t \left(\frac{dx}{d\tau}\right)^2 d\tau\right]$$

- COMPARE WITH THE QM PATH INTEGRAL:

$$-\frac{1}{4D}\int_0^t \left(\frac{dx}{d\tau}\right)^2 d\tau \longleftrightarrow \frac{i}{\hbar}\int_0^t \frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 d\tau$$

$$D \longleftrightarrow \frac{\hbar^2}{2m}$$

$$t \longleftrightarrow \frac{i}{\hbar}t$$

PROPAGATOR.

$$\langle x|\, e^{-\frac{i}{\hbar}Ht}\,|x_0\rangle$$

$$\boxed{G(x,t\,|\,x_0,0) = \langle x|\, e^{-Ht}\,|x_0\rangle}$$

where, $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ is the quantum Hamiltonian of free particle, and $\frac{\hbar^2}{2m} = D$.

<u>REMEMBER FROM Q.M.</u>

FOR FREE PARTICLE: $\langle k|x\rangle \equiv \psi_k(x) = \frac{1}{\sqrt{2\pi}}e^{ikx}$, $E_k = \frac{\hbar^2}{2m}k^2 = Dk^2$

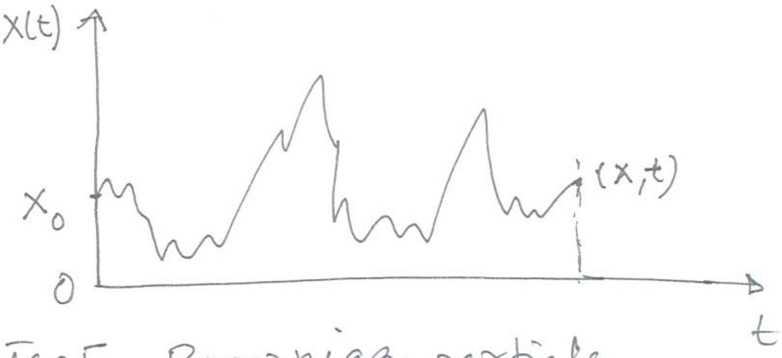
$$\Rightarrow G(x,t\,|\,x_0,0) = \langle x|\, e^{-Ht}\,|x_0\rangle$$

$$= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \langle x|k\rangle \langle k|\, e^{-Ht}\,|k\rangle \langle k|x_0\rangle$$

$$= \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-ikx}\, e^{-Dk^2t}\, e^{ikx_0} = \frac{e^{-\frac{(x-x_0)^2}{4Dt}}}{\sqrt{4\pi Dt}}$$

SURVIVAL PROBABILITY & FIRST-PASSAGE TIME

- $\dfrac{dx}{dt} = \eta(t)$

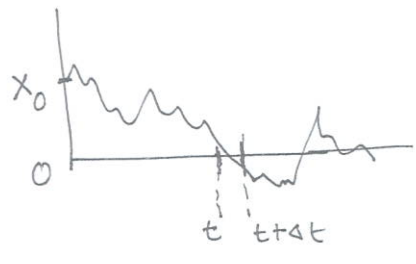


- $S(x_0,t)$ = Probability that Brownian particle starting with x_0 at $t=0$, does not cross origin up to time t.

$$= \int_0^\infty \underbrace{G_A(x,t|x_0,0)}\, dx .$$

↳ PROPAGATOR from x_0 to x without crossing origin.

- $F(x_0,t)\,dt$ = Prob. that Brownian particle crosses origin for the first time between time t and $t+dt$.



(1) $F(x_0,t)\,dt = S(x_0,t) - S(x_0,t+\Delta t)$.

$$\Rightarrow F(x_0,t) = -\frac{\partial S(x_0,t)}{\partial t}$$

(2) $F(x_0,t)$ is also the rate at which particle deposits to origin.

$$\Rightarrow F(x_0,t) = -J_{diff}\Big|_{x=0} = D\,\frac{\partial G_A(x,t|x_0,0)}{\partial x}\Big|_{x=0}$$

↳ Diffusing current ~~to origin~~. towards origin. (− for decreasing x)

- $G_A(x,t\,|\,x_0,0)$ can be obtained by solving the diffusion equation

$$\frac{\partial G_A}{\partial t} = D\frac{\partial^2 G_A}{\partial x^2}$$

with the absorbing boundary condition at the origin

$$G_A(x,t\,|\,x_0,0)\Big|_{x=0} = 0$$

and, $G_A(x,t\,|\,x_0,0)\Big|_{x\to\infty} = 0 \quad \text{for} \quad t<\infty$

and the initial condition:

$$G_A(x,0\,|\,x_0,0) = \delta(x-x_0).$$

- Finding $G_A(x,t\,|\,x_0,0)$ from path integral.

$$G_A(x,t\,|\,x_0,0) = \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}[x(\tau)]\, \exp\left[-\frac{1}{4D}\int_0^t \left(\frac{dx}{d\tau}\right)^2 d\tau\right] \left\{\prod_{\tau=0}^{t} \theta(x(\tau))\right\}$$

$$\exp\left[\int_0^t d\tau \ln \theta(x(\tau))\right]$$

$$= \langle x|\, e^{-Ht}\,|x_0\rangle$$

with $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

$$\frac{\hbar^2}{2m} = D$$

$$V(x) = \begin{cases} 0 & \text{for } x>0 \\ \infty & \text{for } x\le 0 \end{cases}$$

Eigenfunctions : $\varphi_k(x) = \sqrt{\frac{2}{\pi}}\, \sin kx \quad , \; k \geq 0$

Eigen values : $E_k = \frac{\hbar^2}{2m} k^2 = D k^2$

$$\Rightarrow \quad G_A(x, t \mid x_0, 0) = \frac{2}{\pi} \int_0^\infty \sin(kx) \sin(kx_0)\, e^{-Dk^2 t}\, dk.$$

$$= \frac{1}{\sqrt{4\pi D t}} \left[e^{-\frac{(x-x_0)^2}{4Dt}} - e^{-\frac{(x+x_0)^2}{4Dt}} \right]$$

[Hint : $\sin kx = \frac{1}{2i}\left(e^{ikx} - e^{-ikx}\right)$]

- It is easily verified the G_A satisfies D.E, as each of the terms independently does.

~~at~~ and, $G_A(0, t \mid x_0, 0) = 0 \quad \forall\, t > 0$.

Note: The propagator $G_R(x, t \mid x_0, 0)$ with a reflecting barrier at the origin:

$$\left.\frac{\partial G_R}{\partial x}\right|_{x=0} = 0$$

$$G_R(x, t \mid x_0, 0) = \frac{1}{\sqrt{4\pi D t}} \left[e^{-\frac{(x-x_0)^2}{4Dt}} + e^{-\frac{(x+x_0)^2}{4Dt}} \right]$$

SURVIVAL PROBABILITY

- $$S(x_0,t) = \int_0^\infty G_A(x,t\,|\,x_0,0)\,dx = \mathrm{erf}\left(\frac{x_0}{\sqrt{4Dt}}\right)$$

  where $\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-x^2}\,dx$

- $S(x_0,t) \sim t^{-1/2}$ at long time.

- $S(x_0, t\to\infty) = 0$: PARTICLE ALWAYS GETS ABSORBED in 1D.

FIRST-PASSAGE PROBABILITY:

(1) $$F(x_0,t) = -\frac{\partial S(x_0,t)}{\partial t} = \frac{x_0}{\sqrt{4\pi D t^3}}\, e^{-x_0^2/4Dt}$$

(2) $$F(x_0,t) = D\,\frac{\partial G_A(x,t\,|\,x_0,0)}{\partial x}\bigg|_{x=0} =$$

(3) $$G(0,t\,|\,x_0,0) = \int_0^t F(x_0,t')\,\underbrace{G(0,t\,|\,0,t')}_{=\,G(0,t-t'\,|\,0,0)}\,dt'$$

LAPLACE TRANSFORM.

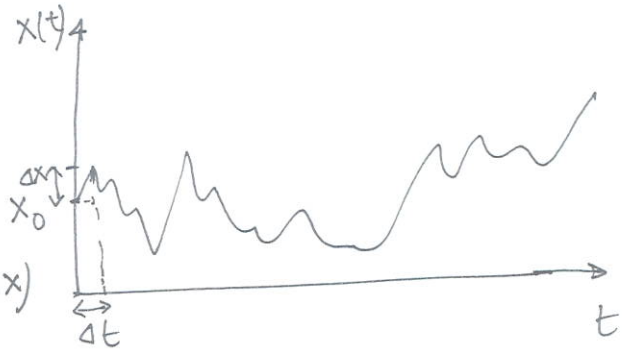
$\Rightarrow$ $$g(0,x_0;s) = f(x_0,s)\cdot g(0,0;s)$$

$\Rightarrow$ $$f(x_0,s) = g(0,x_0;s)/g(0,0;s) = e^{-\frac{x_0}{\sqrt{D}}\sqrt{s}}$$

$$\left[\mathcal{L}^{-1}\left\{e^{-a\sqrt{s}}\right\} = \frac{a}{\sqrt{4\pi t^3}}\,e^{-a^2/4t}\right] \Rightarrow F(x_0,t)$$

BACKWARD FOKKER-PLANCK EQUATION FOR SURVIVAL PROB!

$$\frac{dx}{dt} = \eta(t).$$



$$S(x_0, t+\Delta t) = \int \phi_{\Delta t}(\Delta x)\, \underbrace{S(x_0+\Delta x, t)}_{S(x_0,t) + \Delta x \frac{\partial S}{\partial x_0} + \frac{\Delta x^2}{2}\frac{\partial^2 S}{\partial x_0^2} + \cdots}\, d(\Delta x)$$

$$\langle \Delta x \rangle_{\Delta t} = 0 \quad , \quad \langle \Delta x^2 \rangle_{\Delta t} = 2D\Delta t .$$

$$\Rightarrow \boxed{\frac{\partial S(x_0,t)}{\partial t} = D \frac{\partial^2 S(x_0,t)}{\partial x_0^2}}$$

Derivatives w.r.t initial positions.

Initial condition : $S(x_0, 0) = 1 \quad , \; x_0 > 0$

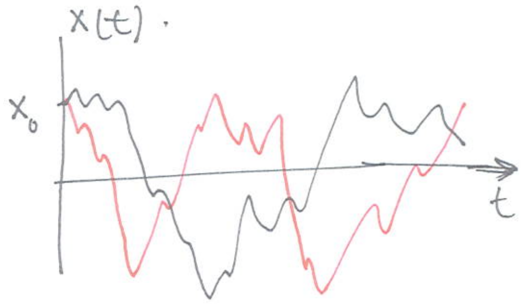
Boundary conditions : $\begin{cases} S(0,t) = 0 \\ S(x_0 \to \infty, t) = 1 . \end{cases}$

It is easily verified that

$$S(x_0,t) = \mathrm{erf}\left(\frac{x_0}{\sqrt{4Dt}}\right),$$ satisfies the above equation with the appropriate initial and boundary conditions.

BROWNIAN FUNCTIONALS: FEYNMAN-KAC FORMULA

$$T = \int_0^t U(x(\tau))\, d\tau$$



↳ RANDOM VARIABLE
WHICH DEPENDS ON REALIZATIONS of $\{x(\tau)\}$.

$$\boxed{P(T, t \mid x_0) = ?}$$

Examples:

(a) $U(x) = -\ln \theta(x)$ ← IN Survival probability

(b) $U(x) = \theta(x)$: $T \to$ occupation time.

Consider the Laplace transform:

$$Q(x_0, t) = \int_0^\infty e^{-\alpha T} P(T, t \mid x_0)\, dT$$

$$= \left\langle e^{-\alpha \int_0^t U(x(\tau))\, d\tau} \right\rangle \quad \text{with } x(0) = x_0 .$$

$$= \int_{-\infty}^{+\infty} dx \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}[x(\tau)] \exp\left[-\frac{1}{4D}\int_0^t d\tau \left(\frac{dx}{d\tau}\right)^2\right] \exp\left[-\alpha \int_0^t U(x(\tau))\, d\tau\right]$$

$t \to \frac{i}{\hbar} t$

$D \to \frac{\hbar^2}{2m}$

$$= \int_{-\infty}^{+\infty} dx \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}[x(\tau)] \exp\left[\frac{i}{\hbar}\int_0^t \underline{L(\dot{x}, x, \tau)}\, d\tau\right]$$

↳ K.E − P.E (Langrangian)
$= \frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 - \alpha U(x)$.

$\frac{i}{\hbar} t \to t$

$$= \int_{-\infty}^{+\infty} dx \underbrace{\langle x | e^{-Ht} | x_0 \rangle}_{G(x, t \mid x_0, 0)}$$

$$\langle x| e^{-Ht} |x_0\rangle = G(x,t|x_0,0)$$

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \alpha U(x).$$

$G(x,t|x_0,0)$ satisfies the schrödinger equation

$$\boxed{\frac{\partial G}{\partial t} = D\frac{\partial^2 G}{\partial x^2} - \alpha U(x) G}$$

$$\begin{cases} \frac{i}{\hbar}t \to t \\ \frac{\hbar^2}{2m} \to D. \end{cases}$$

with the initial condition $G(x,0|x_0,0) = \delta(x-x_0)$

Proof:

$$G(x,t|x_0,0) = \langle x| e^{-Ht} |x_0\rangle$$

$$= \int dn \, \langle x|n\rangle \langle n| e^{-Ht} |n\rangle \langle n|x_0\rangle$$

$$= \int dn \, \psi_n^*(x) \, e^{-E_n t} \, \psi_n^*(x_0)$$

{ Energy eigenstates}

$$-\frac{\partial G}{\partial t} = \int dn \, \psi_n^*(x) \, E_n \, e^{-E_n t} \, \psi_n^*(x_0).$$

$$\Big[-\underset{\substack{\| \\ D.}}{\left(\frac{\hbar^2}{2m}\right)}\frac{\partial^2}{\partial x^2} + s U(x)\Big] G = HG = \int dn \left[H\psi_n^*(x)\right] e^{-E_n t} \psi_n^*(x_0)$$

$$= \int dn \, E_n \psi_n^*(x) \, e^{-E_n t} \psi_n^*(x_0)$$

$$\Rightarrow -\frac{\partial G}{\partial t} = \left[-D\frac{\partial^2}{\partial x^2} + \alpha U(x)\right] G$$

$$\Rightarrow \frac{\partial G}{\partial t} = D\frac{\partial^2 G}{\partial x^2} - \alpha U(x).$$

$$\to Q(x_0,t) = \int_{-\infty}^{+\infty} dx \, G(x,t|x_0,0)$$

BACKWARD FOKKER-PLANCK EQUATION:

$$G(x,t\,|\,x_0,0) = \langle x|\,e^{-Ht}\,|x_0\rangle = \int dn\, \psi_n(x)\, e^{-E_n t}\, \psi_n^*(x_0).$$

$$\Rightarrow \Big[-\underbrace{D}_{=\frac{\hbar^2}{2m}}\frac{\partial^2}{\partial x_0^2} + sU(x_0)\Big]\, G = H_{x_0} G = \int dn\, \psi_n(x)\, e^{-E_n t}\,\big[H_{x_0}\psi_n^*(x_0)\big]$$

$$= \int dn\, \psi_n(x)\, e^{-E_n t}\, E_n\, \psi_n^*(x_0).$$

$$\Rightarrow \frac{\partial G}{\partial t} = \underbrace{D\frac{\partial^2 G}{\partial x_0^2} - \alpha U(x_0)\, G(x,t\,|\,x_0,0)}_{\downarrow}.$$

$$\int_{-\infty}^{+\infty} dx\,\Big[\qquad\qquad\Big]$$

$$\Downarrow$$

$$\boxed{\frac{\partial Q}{\partial t} = D\frac{\partial^2 Q}{\partial x_0^2} - \alpha U(x_0)\, Q(x_0,t).} \qquad Q(x_0,0) = 1.$$

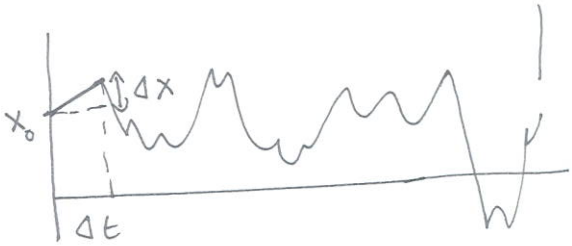
Boundary conditions depend on the behavior of $U(x)$ at large x.

Another Laplace transform: $\tilde{Q}(x_0) = \int_0^\infty e^{-st}\, Q(x_0,t)\, dt.$

$$\boxed{D\frac{d^2\tilde{Q}}{dx_0^2} - \big[s + \alpha U(x_0)\big]\,\tilde{Q}(x_0) = -1}.$$

ANOTHER DERIVATION OF BACKWARD FOKKER-PLANCK EQ:

$$Q(x_0,t) = \left\langle e^{-\alpha\int_0^t U(x(\tau))\,d\tau} \right\rangle \quad , \quad x(0) = x_0 .$$



$$Q(x_0,t+\Delta t) = \left\langle e^{-\alpha\int_0^{t+\Delta t} U(x(\tau))\,d\tau} \right\rangle$$

$$= \left\langle \underbrace{e^{-\alpha\int_0^{\Delta t} U(x(\tau))\,d\tau}}_{\substack{\downarrow\ \Delta t \text{ small} \\ [1-\alpha\Delta t\,U(x_0)]}} \cdot \underbrace{e^{-\alpha\int_{\Delta t}^{t+\Delta t} U(x(\tau))\,d\tau}}_{\substack{\downarrow \\ Q(x_0+\Delta x,\,t)}} \cdot \right\rangle$$

$$Q(x_0,t+\Delta t) \approx [1-\alpha\Delta t\,U(x_0)] \left\langle Q(x_0+\Delta x,t)\right\rangle_{\Delta x}$$

For small Δt ·

$$= [1-\alpha\Delta t\,U(x_0)]\left[Q(x_0,t) + \langle\Delta x\rangle \frac{\partial Q}{\partial x_0} + \frac{\langle\Delta x^2\rangle}{2}\frac{\partial^2 Q}{\partial x_0^2} + \cdots\right]$$

$$= [1-\alpha\Delta t\,U(x_0)]\left[Q(x_0,t) + D\Delta t\frac{\partial^2 Q}{\partial x_0^2} + \cdots\right]$$

$$= Q(x_0,t) + D\frac{\partial^2 Q}{\partial x_0^2}\cdot\Delta t - \alpha\Delta t\,U(x_0)\,Q(x_0,t) + \cdots$$

$$\Rightarrow \lim_{\Delta t\to 0} \frac{Q(x_0,t+\Delta t) - Q(x_0,t)}{\Delta t} = D\frac{\partial^2 Q}{\partial x_0^2} - \alpha U(x_0)\,Q(x_0,t)$$

or,

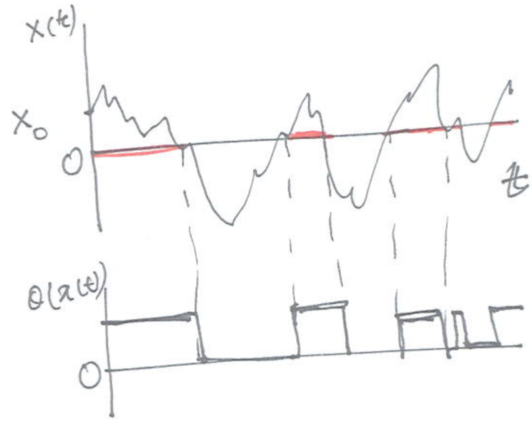
$$\boxed{\frac{\partial Q}{\partial t} = D\frac{\partial^2 Q}{\partial x_0^2} - \alpha\, U(x_0)\, Q(x_0,t)}\,.$$

OCCUPATION TIME : LÉVY'S ARCSINE LAW

$$T = \int_0^t \theta\left[x(\tau)\right] d\tau \quad , \quad U(x) = \theta(x).$$

↳ Total time spent on the positive side (CUMULATIVE)

$$P(T, t \mid x_0) = ?$$



$$\tilde{Q}(x_0) = \int_0^\infty dt\, e^{-st} \int_0^\infty dT\, e^{-\alpha T}\, P(T, t \mid x_0).$$

$$\boxed{D \frac{d^2 \tilde{Q}}{dx_0^2} - \left[s + \alpha\,\theta(x_0)\right] \tilde{Q} = -1}.$$

B.C. $x_0 \to \infty \Rightarrow T \to t$, i.e. $P(T, t \mid \infty) = \delta(T - t)$.

$x_0 \to -\infty \Rightarrow T \to 0$, i.e. $P(T, t \mid -\infty) = \delta(T)$.

$$\Rightarrow \left.\begin{aligned} \tilde{Q}(x_0 \to \infty) &= \frac{1}{s+\alpha} \\ \tilde{Q}(x_0 \to -\infty) &= \frac{1}{s} \end{aligned}\right\} \text{Boundary conditions.}$$

- For $x_0 > 0$: $\quad D \dfrac{d^2 \tilde{Q}}{dx_0^2} - (s + \alpha)\tilde{Q} = -1$

- For $x_0 < 0$: $\quad D \dfrac{d^2 \tilde{Q}}{dx_0^2} - s\tilde{Q} = -1.$

Solutions:

For $x_0 > 0$: $\tilde{Q}(x_0) = \dfrac{1}{s+\alpha} + A\, e^{-\sqrt{s+\alpha}\,\frac{x_0}{\sqrt{D}}}$.

For $x_0 < 0$: $\tilde{Q}(x_0) = \dfrac{1}{s} + B\, e^{\sqrt{\alpha}\cdot\frac{x_0}{\sqrt{D}}}$.

At $x_0 = 0$:

$$\begin{cases} \tilde{Q}(0^+) = \tilde{Q}(0^-) \;\longrightarrow\; \dfrac{1}{s+\alpha} + A = \dfrac{1}{s} + B \\[2ex] \left.\dfrac{d\tilde{Q}}{dx_0}\right|_{x_0=0^+} = \left.\dfrac{d\tilde{Q}}{dx_0}\right|_{x_0=0^-} \;\longrightarrow\; -\dfrac{\sqrt{s+\alpha}}{\sqrt{D}}\,A = \dfrac{\sqrt{\alpha}}{\sqrt{D}}\,B. \end{cases}$$

$$\Rightarrow \begin{cases} A = \dfrac{1}{\sqrt{s}\,\sqrt{s+\alpha}} - \dfrac{1}{s+\alpha} \\[2ex] B = \dfrac{1}{\sqrt{s}\,\sqrt{s+\alpha}} - \dfrac{1}{s} \end{cases}$$

- $\tilde{Q}(0) = \dfrac{1}{\sqrt{s}\,\sqrt{s+\alpha}}$.

$$\Rightarrow P(T,t|0) = \frac{1}{\pi}\,\frac{1}{\sqrt{T(t-T)}}$$

- $\displaystyle\int_0^T P(T',t|0)\,dT' = \frac{2}{\pi}\arcsin\left(\sqrt{\frac{T}{t}}\right)$.

$\to$ Lévy's arcsine Law.

$\cancel{\mathcal{L}_s^{-1}\left\{\dfrac{1}{\sqrt{s+\alpha}}\right\} = \dfrac{e^{-\alpha t}}{\sqrt{\pi t}}}$

$$\mathcal{L}_\alpha^{-1}\left\{\frac{1}{\sqrt{\alpha+s}}\right\} = \frac{e^{-sT}}{\sqrt{\pi T}}$$

$$\mathcal{L}_s^{-1}\left\{e^{-sT}\right\} = \delta(t-T).$$

$$\Rightarrow \mathcal{L}_s^{-1}\left\{\frac{e^{-st}}{\sqrt{s}}\right\} = \int_0^t \delta(t'-T)\,\frac{dt'}{\sqrt{\pi(t-t')}}$$

$$= \frac{1}{\sqrt{\pi}\,\sqrt{t-T}}$$

BROWNIAN MOTION IN EXTERNAL POTENTIAL:

LANGEVIN EQ: (OVERDAMPED).

$$\frac{dx}{dt} = \frac{F(x)}{\gamma} + \eta(t).$$

$$m\frac{d^2x}{dt^2} = -\gamma\frac{dx}{dt} + F(x) + \eta$$

$$F(x) = -U'(x) \quad , \quad \langle \eta(t) \rangle = 0 \quad , \quad \langle \eta(t)\eta(t') \rangle = 2D\delta(t-t')$$

$$\Delta x(t) \approx \frac{1}{\gamma} F(x)\Delta t + \int_t^{t+\Delta t} \eta(\tau)\, d\tau .$$

$$\langle \Delta x \rangle = \frac{F(x)}{\gamma}\Delta t + o(\Delta t) \leftarrow$$ terms higher order in Δt

$$\langle \Delta x^2 \rangle = 2D\Delta t + o(\Delta t).$$

$$P(x, t+\Delta t) = \int_{-\infty}^{+\infty} \underbrace{P(x-\Delta x, t)\ \phi_{\Delta t}(\Delta x | x-\Delta x)}_{= f(x-\Delta x)}\, d(\Delta x).$$

$$f(x-\Delta x) = f(x) - \Delta x\, f'(x) + \frac{(\Delta x)^2}{2} f''(x) + \cdots$$

$$\Rightarrow P(x, t+\Delta t) = \int_{-\infty}^{+\infty} d(\Delta x) \Big\{ P(x,t)\, \phi_{\Delta t}(\Delta x | x) - \Delta x \frac{\partial}{\partial x}\left[P(x,t)\, \phi_{\Delta t}(\Delta x | x)\right] + \frac{\Delta x^2}{2}\frac{\partial^2}{\partial x^2}\left[P(x,t)\, \phi_{\Delta t}(\Delta x | x)\right] + \cdots \Big\}$$

Integration over Δx can be taken inside the derivatives w.r.t x, as they are independent.

$$\int_{-\infty}^{+\infty} (\Delta x)^n \, \phi_{\Delta t}(\Delta x | x) \, d(\Delta x) = \langle (\Delta x)^n \rangle$$

$$\Rightarrow P(x, t+\Delta t) = P(x,t) - \frac{\partial}{\partial x}\left[\langle \Delta x \rangle P\right] + \frac{\partial^2}{\partial x^2}\left[\frac{\langle (\Delta x)^2 \rangle}{2} P\right] + \cdots$$

$$\Rightarrow \boxed{\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}\Big[\underbrace{\frac{F(x)}{\gamma} P}_{\text{Drift current}}\Big] + \frac{\partial^2}{\partial x^2}\left[D P\right]}$$

Drift current.

FOR CONSTANT D:

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}\left[\frac{F(x)}{\gamma} P\right] + D \frac{\partial^2 P}{\partial x^2}$$

GENERALIZATION TO N VARIABLES:

$$\bar{x} = (x_1, x_2, \cdots x_N) \qquad P(x_1, x_2 \cdots x_N, t).$$

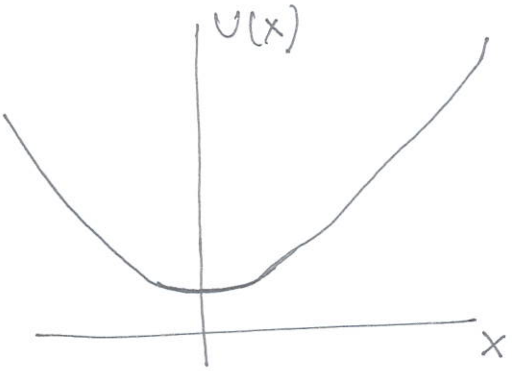
$$\frac{\partial P}{\partial t} = \left[-\sum_{i=1}^{N} \frac{\partial}{\partial x_i} D_i^{(1)}(\{x\}) + \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{\partial^2}{\partial x_i \partial x_j} D_{ij}^{(2)}(\{x\}) \right] P.$$

where,

$$D_i^{(1)} = \frac{\langle \Delta x_i \rangle}{\Delta t}, \quad \Delta t \to 0.$$

$$D_{ij}^{(2)} = \frac{\langle \Delta x_i \Delta x_j \rangle}{\Delta t}, \quad \Delta t \to 0.$$

STATIONARY SOLUTION OF FP EQ. FOR STABLE POTENTIAL:



$U(x) \to \infty$ as $|x| \to 0$.

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x}\left[\frac{1}{\gamma}\frac{dU}{dx}P + D\frac{\partial P}{\partial x}\right], \qquad \left.\begin{array}{l} P(x) \to 0 \\ \frac{\partial P(x,t)}{\partial x} \to 0 \end{array}\right\} \text{as } |x| \to \infty$$

At $t \to \infty$, $\frac{\partial P}{\partial t} \to 0$ ~~stationary~~ $P(x,t) \longrightarrow P_{ss}(x)$.

STATIONARY STATE.

$$\frac{d}{dx}\left[\frac{1}{\gamma}\frac{dU}{dx}P_{ss} + D\frac{dP_{ss}}{dx}\right] = 0$$

$$\Rightarrow \frac{1}{\gamma}\frac{dU}{dx}P_{ss} + D\frac{dP_{ss}}{dx} = \text{constant} = 0 \quad \left(\begin{array}{l}\text{From} \\ \text{Boundary} \\ \text{conditions}\end{array}\right)$$

$$\Rightarrow P_{ss}(x) = P(0)\, e^{-\frac{1}{\gamma D}U(x)}$$

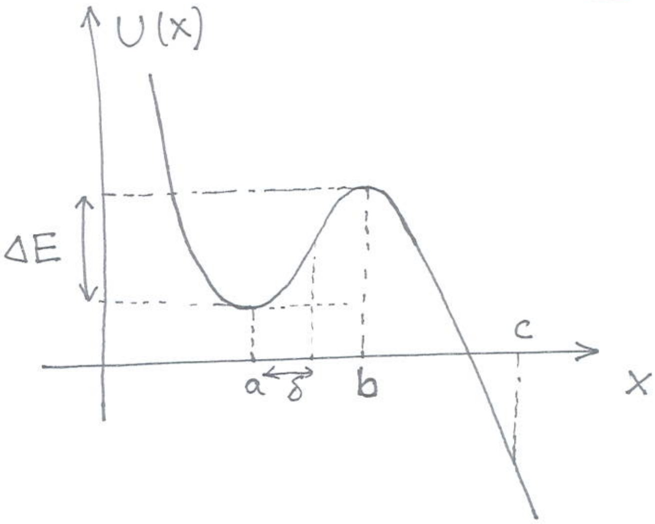
$$\int_{-\infty}^{+\infty} P_{ss}(x)\, dx = 1 \Rightarrow P(0) = \frac{1}{Z}, \quad Z = \int_{-\infty}^{+\infty} e^{-\frac{1}{\gamma D}U(x)} dx$$

$\gamma D = k_B T$. (Einstein relation).

$$\Rightarrow P_{ss}(x) = \frac{1}{Z} e^{-U(x)/k_B T}.$$

$\longleftarrow$ equilibrium distribution.

KRAMER'S ESCAPE OVER A POTENTIAL BARRIER:



$$\frac{\partial P}{\partial t} = -\frac{\partial J}{\partial x}$$

$$J = -\left[\frac{1}{\gamma} U'(x) P + D\frac{\partial P}{\partial x}\right]$$

$$= -D\left[\frac{U'(x)}{k_B T} P + \frac{\partial P}{\partial x}\right]$$

$$= -D\, e^{-\frac{U(x)}{k_B T}} \frac{\partial}{\partial x}\left[e^{\frac{U(x)}{k_B T}} P(x)\right]$$

At equilibrium (ie. if $\Delta E \to \infty$), $\frac{\partial P}{\partial t} = 0$

$$\Rightarrow P(x) = \text{const.}\; e^{-\frac{U(x)}{k_B T}}.$$

, $\text{const.} = P(a)\, e^{\frac{U(a)}{k_B T}}.$

or, $P(x) = P(a)\, e^{-[U(x)-U(a)]/k_B T}.$

But the system is not in equilibrium. ($\Delta E < \infty$)
However, for large $\frac{\Delta E}{k_B T}$, it is near equilibrium: near $x = a$, and there is nonzero current J across $x = b$.

$$\frac{\partial P}{\partial t} \approx 0 \Rightarrow J \text{ is independent of } x.$$

$$\frac{\partial}{\partial x}\left[e^{\frac{U(x)}{k_BT}} P(x)\right] = -\frac{J}{D} e^{\frac{U(x)}{k_BT}}$$

Integrating from $x=a$ to $x=c$, and putting $P(c)\approx 0$

$$- e^{\frac{U(a)}{k_BT}} P(a) = -\frac{J}{D}\int_a^c e^{\frac{U(x)}{k_BT}}\, dx$$

$$\Rightarrow \boxed{J = D\,P(a)\,\frac{e^{\frac{U(a)}{k_BT}}}{\int_a^c e^{\frac{U(x)}{k_BT}}\,dx}}$$

Now $J = \rho R$, R is escape rate

$\rho :=$ Prob. of finding a particle inside the well near $x=a$.

$$= \int_{a-\delta}^{a+\delta} P(x)\,dx \approx P(a)\int_{a-\delta}^{a+\delta} e^{-[U(x)-U(a)]/k_BT}\,dx.$$

For small k_BT, the integral ~~the~~ is dominated by contribution coming from ~~the behavior~~ around $x=a$. Similarly the integral in the denominator of J above is dominated by contribution from near $x=b$.

Near $x=a$: $\quad U(x) \approx U(a) + \frac{1}{2} U''(a)\, x^2$

Near $x=b$: $\quad U(x) \approx U(b) - \frac{1}{2} |U''(b)|\, x^2$

- $$\rho \approx P(a) \int_{-\infty}^{+\infty} e^{-\frac{1}{2}\frac{U''(a)}{k_B T} x^2} dx = \sqrt{2\pi}\left(\frac{U''(a)}{k_B T}\right)^{-1/2}$$

[~~ex~~ integration range is extended to $\pm\infty$]

- $$\int_a^c e^{\frac{U(x)}{k_B T}} dx \approx e^{\frac{U(b)}{k_B T}} \int_{-\infty}^{+\infty} e^{-\frac{1}{2}\frac{|U''(b)|}{k_B T} x^2} dx$$

$$= e^{\frac{U(b)}{k_B T}} \cdot \sqrt{2\pi} \left(\frac{|U''(b)|}{k_B T}\right)^{-1/2}.$$

$$J = D\, P(a) \frac{1}{\sqrt{2\pi}} \left[\frac{|U''(b)|}{k_B T}\right]^{1/2} e^{-[U(b)-U(a)]/k_B T}$$

$$R = \frac{J}{\rho} = \frac{1}{2\pi\gamma} \sqrt{U''(a)\,|U''(b)|}\; e^{-\frac{\Delta E}{k_B T}}$$

$$\left[\frac{D}{k_B T} = \frac{1}{\gamma}\right]$$

$$\Delta E = U(b) - U(a)$$

$$[\,\Delta E \gg k_B T\,]$$

ORNSTEIN – UHLENBECK PROCESS:

BROWNIAN MOTION IN HARMONIC POTENTIAL.

$$U(x) = \frac{1}{2} \lambda x^2 .$$

OVERDAMPED LANGEVIN EQ:

$$\frac{dx}{dt} = -\frac{\lambda}{\gamma} x + \eta(t) .$$

$\eta(t)$ is Gaussian white noise: $\langle \eta(t) \rangle = 0$

$$\langle \eta(t)\, \eta(t') \rangle = 2D\,\delta(t-t')$$

$$x(t) = x_0\, e^{-\nu t} + \int_0^t e^{-\nu(t-t')}\, \eta(t')\, dt' \quad , \quad \nu = \lambda/\gamma .$$

Since $x(t)$ is linear in η; which is Gaussian.

$$P(x,t) = \frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$

where $\mu = \langle x(t) \rangle$

$$\sigma^2 = \langle x^2(t) \rangle - \langle x(t) \rangle^2$$

$$\langle x(t) \rangle = x_0\, e^{-\nu t}$$

$$\langle x^2(t) \rangle = \underbrace{x_0^2\, e^{-2\nu t}}_{\langle x(t) \rangle^2} + \int_0^t dt_1 \int_0^t dt_2\, e^{-\nu(t-t_1)}\, e^{-\nu(t-t_2)} \times 2D\,.\,\delta(t_1 - t_2) .$$

$$\sigma^2 = 2D \int_0^t dt_1\, e^{-2\nu(t-t_1)} = \frac{\cancel{2}D}{\cancel{2}\nu}\left[1 - e^{-2\nu t}\right] =$$

$$G(x,t\,|\,x_0,0) \equiv P(x,t)$$

$$= \frac{1}{\sqrt{2\pi \frac{D}{\nu}\left(1-e^{-2\nu t}\right)}} \exp\left[-\frac{\left(x - x_0 e^{-\nu t}\right)^2}{\frac{2D}{\nu}\left(1-e^{-2\nu t}\right)}\right]$$

$\nu = \lambda/\gamma$.

<u>Limits:</u>

(a) $t \to \infty$

$$P(x) = \frac{1}{\sqrt{2\pi (D/\nu)}}\, e^{-\frac{1}{2}\lambda x^2/k_B T}, \quad \gamma D = k_B T.$$

$$= \frac{e^{-\cancel{\beta} U(x)/k_B T}}{Z} \quad \text{equilibrium dist}^n.$$

(b) $\lambda \to 0$:

$$\frac{1}{\nu}\left(1-e^{-2\nu t}\right) \longrightarrow 2t.$$

$$G(x,t\,|\,x_0,0) \Longrightarrow \frac{1}{\sqrt{4\pi D t}}\, e^{-\frac{(x-x_0)^2}{4Dt}}$$

FREE BROWNIAN MOTION.

$f_0(x,x_0)$

<u>EXPANSION:</u>

$$G(x,t\,|\,x_0,0) = \sum_{n=0}^{\infty} e^{-\mu_n t} f_n(x,x_0), \quad \mu_0 = 0,\ \mu_n > 0 \text{ for } n>0$$

[WE WILL COME BACK TO IT]

FOKKER-PLANCK TO SCHRÖDINGER EQUATION:

$$\frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial x^2} + \frac{\partial}{\partial x}\left[\frac{U'(x)}{\gamma} P\right]$$

$$= D\frac{\partial^2 P}{\partial x^2} + \frac{U'(x)}{\gamma}\frac{\partial P}{\partial x} + \frac{U''(x)}{\gamma} P. \quad \text{—(1)}$$

THE AIM IS TO GET RID OF THE FIRST DERIVATIVE TERM IN X, AS SCHRÖDINGE EQUATION DOES NOT HAVE A SIMILAR TERM.

- SCHRÖDINGER EQ:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi = i\hbar\frac{\partial \psi}{\partial t}. \quad \text{—(2)}$$

$$\Rightarrow \left[\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - V(x)\right]\psi(x,t) = \frac{\partial \psi}{\partial(\frac{i}{\hbar}t)}.$$

$$\frac{\hbar^2}{2m} \to D, \quad \frac{i}{\hbar}t \to t.$$

$$\Rightarrow \quad \frac{\partial \psi}{\partial t} = \left[D\frac{\partial^2}{\partial x^2} - V(x)\right]\psi(x,t). \quad \text{—— (3)}.$$

NOW, Let $P(x,t) = \phi(x)\,\psi(x,t)$.

$$\frac{\partial P}{\partial x} = \phi'(x)\,\psi(x,t) + \phi(x)\frac{\partial \psi}{\partial x}.$$

$$\frac{\partial^2 P}{\partial x^2} = \phi''(x)\,\psi(x,t) + \phi'(x)\frac{\partial \psi}{\partial x} + \phi'(x)\frac{\partial \psi}{\partial x} + \phi(x)\frac{\partial^2 \psi}{\partial x^2}$$

$$\frac{\partial^2 P}{\partial x^2} = \phi''(x)\,\psi(x,t) + 2\phi'(x)\frac{\partial \psi}{\partial x} + \phi(x)\frac{\partial^2 \psi}{\partial x^2}$$

Substitute in (1) $\Rightarrow$.

$$\phi(x)\frac{\partial \psi}{\partial t} = D\left[\phi''(x)\,\psi(x,t) + 2\phi'(x)\frac{\partial \psi}{\partial x} + \phi(x)\frac{\partial^2 \psi}{\partial x^2}\right]$$
$$+ \frac{U'(x)}{\gamma}\left[\phi'(x)\,\psi(x,t) + \phi(x)\frac{\partial \psi}{\partial x}\right]$$
$$+ \frac{U''(x)}{\gamma}\,\phi(x)\,\psi(x,t).$$

$$\Rightarrow \frac{\partial \psi}{\partial t} = D\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial \psi}{\partial x}\left[2D\frac{\phi'(x)}{\phi(x)} + \frac{U'(x)}{\gamma}\right] \cancel{\frac{\phi'(x)}{\phi(x)}}$$
$$+ \psi(x,t)\left[D\frac{\phi''(x)}{\phi(x)} + \frac{U'(x)}{\gamma}\frac{\phi'(x)}{\phi(x)} + \frac{U''(x)}{\gamma}\right]$$

Putting coefficient of $\frac{\partial \psi}{\partial x} = 0$;

$$\frac{\phi'(x)}{\phi(x)} = -\frac{U'(x)}{2\gamma D}.$$

$$\parallel$$

$$\frac{d}{dx}\left[\ln \phi(x)\right]$$

Integrating $\Rightarrow$ $\phi(x) = e^{-\frac{U(x)}{2\gamma D}}$. , $\left[\gamma D = k_B T\right]$

The constant of integration can be absorbed in ψ.

$$\frac{d}{dx}\left[\frac{\phi'(x)}{\phi(x)}\right] = -\frac{U''(x)}{2\gamma D}.$$

$$\Rightarrow \quad \frac{\phi''(x)}{\phi(x)} - \left[\frac{\phi'(x)}{\phi(x)}\right]^2 = -\frac{U''(x)}{2\gamma D}.$$

$$\Rightarrow \quad \frac{\phi''(x)}{\phi(x)} = \left[\frac{U'(x)}{2\gamma D}\right]^2 - \frac{U''(x)}{2\gamma D}.$$

Coefficient of $\psi(x,t)$:

$$\frac{[U'(x)]^2}{4\gamma^2 D} - \frac{U''(x)}{2\gamma} + \frac{U'(x)}{\gamma}\cdot\left(-\frac{U'(x)}{2\gamma D}\right) + \frac{U''(x)}{\gamma}.$$

$$= -\left[\frac{[U'(x)]^2}{4\gamma^2 D} - \frac{U''(x)}{2\gamma}\right]$$

Thus: $$P(x,t) = e^{-\frac{U(x)}{2\gamma D}}\,\psi(x,t)$$ $[\gamma D = k_B T]$

$$\frac{\partial \psi}{\partial t} = \left[D\frac{\partial^2}{\partial x^2} - V(x)\right]\psi(x,t).$$

with $$V(x) = \frac{[U'(x)]^2}{4\gamma^2 D} - \frac{U''(x)}{2\gamma}.$$

PATH INTEGRAL APPROACH:

$$\frac{dx}{dt} = -\frac{U'(x)}{\gamma} + \eta(t).$$

$$P[\{\eta(\tau)\}] \propto \exp\left[-\frac{1}{4D}\int_0^t \eta^2(\tau)\,d\tau\right]$$

$$\Rightarrow P[\{x(\tau)\}] \propto \left|\frac{d\{\eta(\tau)\}}{d\{x(\tau)\}}\right| \exp\left[-\frac{1}{4D}\int_0^t \left[\frac{dx}{d\tau}+\frac{U'(x)}{\gamma}\right]^2 d\tau\right]$$

Jacobian

- $$\int_0^t \left[\frac{dx}{d\tau}+\frac{U'(x)}{\gamma}\right]^2 d\tau.$$

$$= \int_0^t \left[\left(\frac{dx}{d\tau}\right)^2 + \frac{[U'(x)]^2}{\gamma^2} + \frac{2}{\gamma}\frac{dx}{d\tau}U'(x)\right] d\tau.$$

- $$\int_0^t \frac{dx}{d\tau}U'(x(\tau))\,d\tau = \int_0^t \frac{d}{d\tau}\left[U(x(\tau))\right]d\tau = U(x) - U(x_0)$$

$$\begin{cases} x(t) = x \\ x(0) = x_0 \end{cases}$$

$$\Rightarrow \exp\left[-\frac{1}{4D}\int_0^t \left(\frac{dx}{d\tau}+\frac{U'(x)}{\gamma}\right)^2 d\tau\right]$$

$$= \exp\left[-\frac{U(x)-U(x_0)}{2\gamma D}\right]\exp\left[-\frac{1}{4D}\int_0^t\left(\left(\frac{dx}{d\tau}\right)^2+\frac{[U'(x)]^2}{\gamma^2}\right)d\tau\right]$$

THE JACOBIAN :

$$\eta(\tau) = \frac{dx}{d\tau} - \frac{F(x)}{\gamma} \qquad F(x) = -U'(x).$$

DISTRETIZATION :

$$\underset{0}{|}\!\overset{1\ 2\ \cdots\ N}{\text{—+—+—+—+—+—}}\!\underset{t}{|} \qquad \leftrightarrow \ \varepsilon \qquad N\varepsilon = t \qquad \begin{array}{l} \varepsilon \to 0 \\ N \to \infty \end{array}$$

$$\eta_\varepsilon(\tau) = \frac{1}{\varepsilon}\left[x(\tau) - x(\tau-\varepsilon)\right] - \frac{1}{\gamma}\left[\frac{F(x(\tau)) + F(x(\tau-\varepsilon))}{2}\right]$$

$$\frac{\partial \eta_\varepsilon(\tau)}{\partial x(\tau)} = \frac{1}{\varepsilon}\left[1 - \varepsilon\,\frac{F'(x(\tau))}{2\gamma}\right]$$

$$\frac{\partial \eta_\varepsilon(\tau)}{\partial x(\tau-\varepsilon)} = -\frac{1}{\varepsilon}\left[1 + \varepsilon.\,\frac{F'(x(\tau-\varepsilon))}{2\gamma}\right]$$

$$\text{JACOBIAN} = \text{abs}\left|\begin{matrix} \ddots & & 0 \\ \ddots & \ddots & \\ 0 & \ddots & \ddots \end{matrix}\right|$$

$$= \left(\frac{1}{\varepsilon}\right)^N \prod_{\tau}^{N}\left[1 - \varepsilon\,\frac{F'(x(\tau))}{2\gamma}\right]$$

Will be absorbed in normalization

$$\propto \exp \sum_{\tau}^{N} \ln\left(1 - \varepsilon\,\frac{F'(x(\tau))}{2\gamma}\right)$$

$$\left.\begin{array}{l} N \to \infty \\ \varepsilon \to 0 \\ N\varepsilon = t \end{array}\right\}. \longrightarrow \exp\left[-\frac{1}{2\gamma}\int_0^t F'(x(\tau))\,d\tau\right]$$

$$= \exp\left[\frac{1}{2\gamma}\int_0^t U''(x(\tau))\,d\tau\right]$$

$$G(x,t\,|\,x_0,0) = e^{-\frac{[U(x)-U(x_0)]}{2\gamma D}} \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}[x(\tau)]$$

$$\cdot \exp\Bigg[\underbrace{-\frac{1}{4D}\int_0^t d\tau \left[\left(\frac{dx}{d\tau}\right)^2 + \frac{[U'(x)]^2}{\gamma^2} - \frac{4D}{2\gamma}U''(x)\right]}\Bigg]$$

change of variable:

$\tau \to \frac{i}{\hbar}\tau$

$d\tau \to \frac{i}{\hbar}d\tau$

upper limit $\to -i\hbar t$

$$\frac{i}{\hbar}\int_0^{-i\hbar t} d\tau \left[\underbrace{\frac{\hbar^2}{4D}\left(\frac{dx}{d\tau}\right)^2}_{\text{K.E.}} - \underbrace{\left(\frac{[U'(x)]^2}{4\gamma^2 D} - \frac{U''(x)}{2\gamma}\right)}_{\text{P.E.}}\right]$$

$(D = \hbar^2/2m)$.

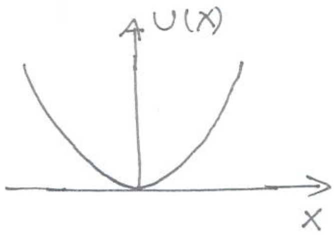
$$\boxed{G(x,t\,|\,x_0,0) = e^{-\frac{[U(x)-U(x_0)]}{2\gamma D}} \langle x|\, e^{-Ht}\,|x_0\rangle}$$

where, $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$ $\quad\left[\frac{\hbar^2}{2m} = D\right]$

with $V = \frac{[U'(x)]^2}{4\gamma^2 D} - \frac{U''(x)}{2\gamma}$.

BROWNIAN MOTION IN HARMONIC POTENTIAL : (OU PROCESS)

$$U(x) = \frac{\lambda}{2} x^2$$



$$U'(x) = \lambda x \quad , \quad U''(x) = \lambda .$$

$$V(x) = \frac{\lambda^2 x^2}{4\gamma^2 D} - \frac{\lambda}{2\gamma} = \frac{1}{2} m\omega^2 x^2 - \frac{\lambda}{2\gamma} .$$

$$\omega^2 = \frac{\lambda^2}{\gamma^2 \, 2mD} \Rightarrow \omega = \frac{\lambda}{\gamma \hbar} . \qquad \frac{\hbar^2}{2m} = D .$$

or, $\boxed{\hbar\omega = \frac{\lambda}{\gamma} .}$

$$\langle x | e^{-Ht} | x_0 \rangle = \sum_{n=0}^{\infty} \langle x | n \rangle \, e^{-E_n t} \, \langle n | x_0 \rangle$$

$$= \sum_{n=0}^{\infty} e^{-E_n t} \, \psi_n(x) \, \psi_n^*(x_0) .$$

$$E_n = \hbar\omega (n + 1/2) - \frac{\lambda}{2\gamma} = \frac{n\lambda}{\gamma} .$$

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-\frac{m\omega}{2\hbar} x^2} H_n\left(\sqrt{\frac{m\omega}{\hbar}} \, x \right)$$

$n = 0, 1, 2 \dots$

$$= \frac{1}{\sqrt{2^n n!}} \left(\frac{\lambda}{2\pi\gamma D} \right)^{1/4} e^{-\frac{\lambda x^2}{4\gamma D}} H_n\left(\sqrt{\frac{\lambda}{2\gamma D}} \, x \right)$$

$$\left[\frac{m\omega}{\hbar} = \frac{\hbar\omega}{2 \cdot \frac{\hbar^2}{2m}} = \frac{1}{2} \frac{\lambda}{\gamma D} . \right]$$

HERMITE POLYNOMIALS:

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}$$

orthogonality: $\displaystyle\int_{-\infty}^{+\infty} H_n(x) H_m(x) e^{-x^2} dx = 2^n n! \sqrt{\pi}\, \delta_{m,n}$

[Check from (1) schrodinger eqn, (2) above expression:

$$H''(x) - 2x H'(x) + 2n H_n(x) = 0$$]

$$\langle x | e^{-Ht} | x_0 \rangle = \sum_{n=0}^{\infty} e^{-E_n t} \frac{1}{2^n n!} \left(\frac{\lambda}{2\pi \gamma D}\right)^{1/2} e^{-\frac{\lambda}{4\gamma D}(x^2+x_0^2)} \cdot H_n\left(\sqrt{\frac{\lambda}{2\gamma D}}\, x\right) H_n\left(\sqrt{\frac{\lambda}{2\gamma D}}\, x_0\right)$$

Thus

$$G(x,t|x_0,0) = e^{-\frac{U(x)-U(x_0)}{2\gamma D}} \langle x | e^{-Ht} | x_0 \rangle$$

$$= e^{-\frac{\lambda}{4\gamma D}(x^2 - x_0^2)} \left(\frac{\lambda}{2\pi\gamma D}\right)^{1/2} e^{-\frac{\lambda}{4\gamma D}(x^2+x_0^2)} \cdot \sum_{n=0}^{\infty} e^{-E_n t} \frac{1}{2^n n!} H_n\left(\sqrt{\frac{\lambda}{2\gamma D}}\, x\right) H_n\left(\sqrt{\frac{\lambda}{2\gamma D}}\, x_0\right)$$

$$\boxed{G(x,t|x_0,0) = \sqrt{\frac{\lambda}{2\pi\gamma D}}\, e^{-\frac{\lambda x^2}{2\gamma D}} \sum_{n=0}^{\infty} \frac{e^{-E_n t}}{2^n n!} H_n\left(\sqrt{\frac{\lambda}{2\gamma D}}\, x\right) H_n\left(\sqrt{\frac{\lambda}{2\gamma D}}\, x_0\right) \qquad E_n = n\frac{\lambda}{\gamma}}$$

$H_0(x) = 1$. Compare the $t \to \infty$ limit with the earlier result.

HERMITE FUNCTIONS:

- $$\phi_n(x) = \frac{1}{\sqrt{2^n\, n!\sqrt{\pi}}}\, e^{-x^2/2}\, H_n(x)$$

- $$\int_{-\infty}^{+\infty} \phi_n(x)\, \phi_m(x)\, dx = \delta_{m,n}$$

- $$\phi_n''(x) + \left(2n+1-x^2\right)\phi_n(x) = 0$$ [Schrödinger equation with $\hbar = m = \omega = 1$]

- $$\sum_{n=0}^{\infty} \epsilon^n\, \phi_n(x)\, \phi_n(y) = \frac{1}{\sqrt{\pi(1-\epsilon^2)}} \exp\left[-\frac{1-\epsilon}{1+\epsilon}\,\frac{(x+y)^2}{4} - \frac{1+\epsilon}{1-\epsilon}\,\frac{(x-y)^2}{4}\right]$$

* [MEHLER'S FORMULA] $(-1 < \epsilon < 1)$

USING THE ABOVE IDENTITY SHOW THAT THE TWO SOLUTIONS WE HAVE OBTAINED FOR THE ORNSTEIN-UHLENBECK PROCESS ARE EQUIVALENT; i.e.

$$\frac{1}{\sqrt{2\pi(D/\nu)\left(1-e^{-2\nu t}\right)}} \exp\left[-\frac{\left(x-x_0\, e^{-\nu t}\right)^2}{2(D/\nu)\left(1-e^{-2\nu t}\right)}\right]$$

$$= \frac{1}{\sqrt{2\pi(D/\nu)}}\, e^{-\frac{\nu x^2}{2D}} \sum_{n=0}^{\infty} \frac{e^{-n\nu t}}{2^n\, n!}\, H_n\left(\sqrt{\tfrac{\nu}{2D}}\,x\right) H_n\left(\sqrt{\tfrac{\nu}{2D}}\,x_0\right)$$

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* MEHLER'S FORMULA FOR HERMITE POLYNOMIALS:

$$\sum_{n=0}^{\infty} \frac{H_n(x)\, H_n(y)}{n!}\left(\frac{w}{2}\right)^n = \frac{1}{\sqrt{1-w^2}} \exp\left[\frac{2xyw - (x^2+y^2)\,w^2}{1-w^2}\right]$$

RANDOM ACCELERATION

$$\frac{d^2x}{dt^2} = \eta(t)$$

$x(0) = 0, \; v(0) = 0.$

$\langle \eta(t) \rangle = 0, \; \langle \eta(t)\eta(t') \rangle = \delta(t-t')$

(NON - MARKOV PROCESS).

$$\left.\begin{aligned} \frac{dx}{dt} &= v(t) \\ \frac{dv}{dt} &= \eta(t) \end{aligned}\right\}$$

MARKOV PROCESS.

$$\lim_{\Delta t \to 0} \left\{ \begin{aligned} &\frac{\langle \Delta x \rangle}{\Delta t} = v, \quad \frac{\langle (\Delta x)^2 \rangle}{\Delta t} = 0 \\ &\frac{\langle \Delta v \rangle}{\Delta t} = 0, \quad \frac{\langle (\Delta v)^2 \rangle}{\Delta t} = 1. \\ &\frac{\langle (\Delta x \, \Delta v) \rangle}{\Delta t} = 0 \end{aligned} \right.$$

$P(x, v, t)$ satisfies:

$$\boxed{\frac{\partial P}{\partial t} = -v \frac{\partial P}{\partial x} + \frac{1}{2} \frac{\partial^2 P}{\partial v^2}}$$

WE WILL USE THE GAUSSIAN PROPERTY OF η:

$$v(t) = \frac{dx}{dt} = \int_0^t \eta(t')\, dt'$$

$$x(t) = \int_0^t dt' \int_0^{t'} \eta(t'')\, dt''.$$

$\Rightarrow \langle v(t) \rangle = 0, \quad \langle x(t) \rangle = 0, \quad \langle v^2(t) \rangle = t$

$$\left.\begin{aligned} \langle x(t)\, v(t) \rangle &= \frac{t^2}{2} \\ \langle x^2(t) \rangle &= \frac{t^3}{3} \end{aligned}\right\} \quad \underline{\text{CHECK}}.$$

$$\Sigma = \begin{pmatrix} \langle X^2(t)\rangle & \langle X(t)V(t)\rangle \\ \langle X(t)V(t)\rangle & \langle V^2(t)\rangle \end{pmatrix} = \begin{pmatrix} \frac{t^3}{3} & \frac{t^2}{2} \\ \frac{t^2}{2} & t \end{pmatrix}$$

$$P(x,v,t) = \frac{1}{2\pi |\Sigma|^{1/2}} \exp\left[-\frac{1}{2}(x,v)\,\Sigma^{-1}(x,v)^T\right]$$

$$|\Sigma| = \frac{t^4}{12}$$

$$\Sigma^{-1} = \frac{12}{t^4}\begin{pmatrix} t & -t^2/2 \\ -t^2/2 & t^3/3 \end{pmatrix}$$

$$\frac{1}{2}(x \;\; v)\,\Sigma^{-1}\begin{pmatrix} x \\ v \end{pmatrix} = \frac{6x^2}{t^3} + \frac{2v^2}{t} - \frac{6xv}{t^2}$$

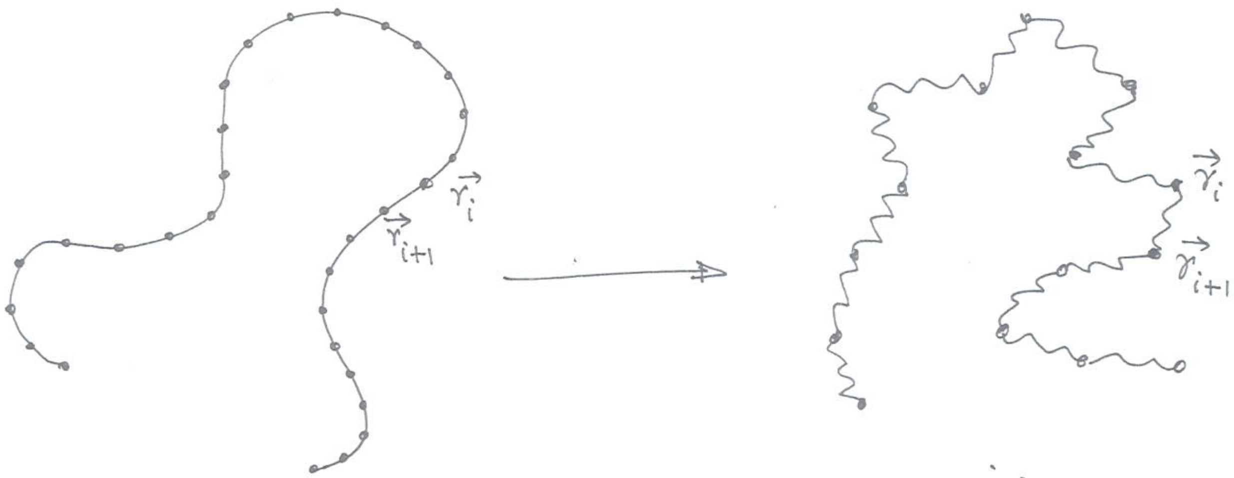
$$P(x,v,t) = \frac{\sqrt{3}}{\pi t^2}\exp\left[-\left(\frac{6x^2}{t^3} + \frac{2v^2}{t} - \frac{6xv}{t^2}\right)\right]$$

$$P_1(x,t) = \int_{-\infty}^{+\infty} P(x,v,t)\,dv$$

$$= \frac{1}{\sqrt{2\pi(t^3/3)}}\exp\left[-\frac{1}{2}\frac{x^2}{(t^3/3)}\right] \qquad \left(\langle x^2\rangle = \frac{t^3}{3}\right.$$

[CHECK THAT THE SOLUTION $P(x,v,t)$ SATISFIES THE FOKKER-PLANCK EQUATION.]

THE ROUSE MODEL OF FLEXIBLE POLYMERS:



REAL POLYMER CHAIN

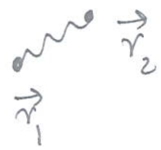
ROUSE CHAIN:
[MONOMERS CONNECTED BY HARMONIC SPRINGS.]

- THE INTER-MONOMER DISTANCE IS FIXED $= a$

- THE INTER-MONOMER DISTANCE IS NOT FIXED.
  HOWEVER, WE FIX:
  $$\left\langle \left(\vec{r}_{i+1} - \vec{r}_{i}\right)^2 \right\rangle = a^2$$

FIRST CONSIDER TWO MONOMERS CONNECTED BY A HARMONIC SPRING: (SPRING CONSTANT $= \lambda$)

$$U(\vec{r}_1, \vec{r}_2) = \frac{\lambda}{2} \left(\vec{r}_2 - \vec{r}_1\right)^2$$



$\vec{r}_i = (x_i, y_i, z_i)$

$$= \frac{\lambda}{2} \left[(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2 \right]$$

LANGEVIN EQUATION:

$$\frac{d\vec{r}_i}{dt} = -\frac{1}{\gamma} \vec{\nabla}_i U + \vec{\eta}_i$$

$$\vec{\eta}_i \equiv \left(\eta_i^{(x)}, \eta_i^{(y)}, \eta_i^{(z)} \right)$$

$$\left\langle \eta_i^{(\alpha)}(t) \right\rangle = 0$$

$$\left\langle \eta_i^{(\alpha)}(t)\, \eta_j^{(\alpha')}(t') \right\rangle = \delta_{ij}\, \delta_{\alpha,\alpha'} \cdot 2D\, \delta(t - t')$$

Let us look at the x-component:

$$\frac{dx_1}{dt} = \frac{\lambda}{\gamma}(x_2 - x_1) + \eta_1^{(x)}$$

$$\frac{dx_2}{dt} = -\frac{\lambda}{\gamma}(x_2 - x_1) + \eta_2^{(x)}$$

Let $x_{12} = x_2 - x_1$

$$\frac{dx_{12}}{dt} = -\frac{2\lambda}{\gamma} x_{12} + \xi_x$$

$$\left\{ \begin{array}{l} \xi_x = \eta_2^{(x)} - \eta_1^{(x)} \\ \langle \xi_x \rangle = \langle \eta_2^{(x)} \rangle - \langle \eta_1^{(x)} \rangle = 0 \\ \langle \xi_x(t)\, \xi_x(t') \rangle = 4D\,\delta(t-t'). \end{array} \right.$$

SIMILAR EQS. FOR: y_{12} & z_{12}

ORNSTEIN-UHLENBECK PROCESS: WITH $\lambda \to 2\lambda$, $D \to 2D$.

$$\left. \begin{array}{l} \langle x_{12}^2(t) \rangle \\ \langle y_{12}^2(t) \rangle \\ \langle z_{12}^2(t) \rangle \end{array} \right\} \xrightarrow{t \to \infty} \frac{\gamma D}{\lambda} = \frac{k_B T}{\lambda}.$$

Thus. $$\underbrace{\langle (\vec{r}_2 - \vec{r}_1)^2 \rangle}_{a^2} = \langle x_{12}^2 \rangle + \langle y_{12}^2 \rangle + \langle z_{12}^2 \rangle = 3\frac{k_B T}{\lambda}.$$

$$\Rightarrow \boxed{\lambda = \frac{3k_B T}{a^2}}$$

This ensures that the internal properties (inter-monomer separations) of the chain do not change with changing temperature, as the spring constant changes accordingly.

N BEADS CONNECTED BY HARMONIC SPRINGS:

$\{\vec{r}_i\} \equiv (\vec{r}_1, \vec{r}_2, \cdots \vec{r}_N)$ are the positions of the beads.

$$U(\{\vec{r}_i\}) = \frac{\lambda}{2} \sum_{n=2}^{N} \left(\vec{r}_n - \vec{r}_{n-1} \right)^2$$

$\vec{r}_i \equiv (x_i, y_i, z_i)$

LANGEVIN EQUATION: $\left[\lambda = \frac{3 k_B T}{a^2} \right]$

$\vec{\eta}_i = (\eta_i^{(x)}, \eta_i^{(y)}, \eta_i^{(z)})$

$$(1) \begin{cases} \dfrac{d\vec{r}_n}{dt} = \dfrac{\lambda}{\gamma} \left(\vec{r}_{n+1} + \vec{r}_{n-1} - 2\vec{r}_n \right) + \vec{\eta}_n , \quad n = 2, 3 \cdots N-1 \\[2ex] \dfrac{d\vec{r}_1}{dt} = -\dfrac{\lambda}{\gamma} \left(\vec{r}_1 - \vec{r}_2 \right) + \vec{\eta}_1 \\[2ex] \dfrac{d\vec{r}_N}{dt} = -\dfrac{\lambda}{\gamma} \left(\vec{r}_N - \vec{r}_{N-1} \right) + \vec{\eta}_N . \end{cases}$$

The ~~above~~ above three equations can be combined into one:

$$(2) \quad \boxed{\frac{d\vec{r}_n}{dt} = \frac{\lambda}{\gamma} \left(\vec{r}_{n+1} + \vec{r}_{n-1} - 2\vec{r}_n \right) + \vec{\eta}_n} , \quad n = 1, 2, \cdots N$$

provided we put two fictitious beads 0 and $N+1$, and $\vec{r}_0 = \vec{r}_1$ & $\vec{r}_{N+1} = \vec{r}_N$. (Boundary condition)

DYNAMICS OF THE CENTER OF MASS:

$$\vec{R}_{CM} = \frac{1}{N} \sum_{n=1}^{N} \vec{r}_n$$

Then, $$\boxed{\frac{d\vec{R}_{CM}}{dt} = \vec{\xi}(t)} \; , \quad \vec{\xi} = \frac{1}{N}\sum_{n=1}^{N} \vec{\eta}_n \, .$$

WHICH IS A BROWNIAN MOTION with $\boxed{D_{CM} = \frac{D}{N}}$

$$\langle \xi^{(\alpha)} \rangle = 0$$

$$\langle \xi^{(\alpha)}(t) \xi^{(\alpha')}(t') \rangle = \delta_{\alpha,\alpha'} \frac{2D}{N} \delta(t-t')$$

LONG CHAIN (LARGE N). LIMIT

FOR LARGE N, the bead index n ~~___~~ can be treated as continuous variable. $\left[\frac{\Delta n}{N} = \frac{1}{N} \text{ is small} \right.$

~~$\vec{\xi}(t)$~~

$$(3) \quad \frac{\partial \vec{r}(n,t)}{\partial t} = \frac{\lambda}{\gamma} \frac{\partial^2 \vec{r}}{\partial n^2} + \vec{\eta}(n,t)$$

$$\left[\begin{aligned} & \vec{r}_{n+1} + \vec{r}_{n-1} - 2\vec{r}_n \\ & = \frac{1}{N^2} \cdot \frac{\vec{r}_{n+1} + \vec{r}_{n-1} - 2\vec{r}_n}{(1/N^2)} \\ & \approx \frac{1}{N^2} \frac{\partial^2 \vec{r}}{\partial (n/N)^2} = \frac{\partial^2 \vec{r}}{\partial n^2} \end{aligned} \right.$$

The boundary conditions become:

$$\frac{\partial \vec{r}(n,t)}{\partial n} = 0 \quad \text{at } n=0, \; n=N.$$

$$\langle \eta^{(\alpha)}(n,t) \, \eta^{(\alpha')}(n',t') \rangle = \delta_{\alpha,\alpha'} \, \delta(n-n') \, 2D \delta(t-t')$$

Fourier cosine decomposition:

$$\vec{r}(n,t) = \tilde{r}(0,t) + \sum_{m=1}^{\infty} \tilde{r}(m,t) \cos\left(\frac{m\pi n}{N}\right)$$

$$\left[\frac{\partial \vec{r}}{\partial n} = \sum_{m=1}^{\infty} \tilde{r}(m,t) \cdot \left(-\frac{m\pi}{N}\right) \sin\left(\frac{m\pi n}{N}\right) = 0 \text{ at } n=0,N. \right]$$

$$\tilde{r}(0,t) = \frac{1}{N} \int_0^N \vec{r}(n,t)\, dn \longrightarrow \text{CENTER OF MASS.}$$

$$\tilde{r}(m,t) = \frac{2}{N} \int_0^N \vec{r}(n,t) \cos\left(\frac{m\pi n}{N}\right) dn \quad , \quad m = 1, 2 \cdots$$

$$\left[\frac{2}{\pi} \int_0^{\pi} \cos(mx) \cos(nx)\, dx = \delta_{m,n} \right]$$

~~Each mode evolve independently~~:

Each mode evolve independently:

$$\boxed{\frac{d\tilde{r}(m,t)}{dt} = -\chi_m \tilde{r}(m,t) + \tilde{\eta}(m,t)}$$

OU PROCESS.

$$\chi_m = m^2 \frac{\pi^2}{N^2} \cdot \frac{\lambda}{\gamma} = m^2/\tau_0 \quad , \quad \tau_0 = \frac{N^2 \gamma}{\pi^2 \lambda}$$

$$\tilde{\eta}(m,t) = \frac{2}{N} \int_0^N \vec{\eta}(n,t) \cos\left(\frac{m\pi n}{N}\right) dn$$

$$\left\langle \tilde{\eta}^{(\alpha)}(m,t)\, \tilde{\eta}^{(\alpha')}(m',t') \right\rangle = \left(\frac{2}{N}\right)^2 \int_0^N dn \cos\left(\frac{m\pi n}{N}\right) \int_0^N dn' \cos\left(\frac{m'\pi n'}{N}\right) \cdot \left\langle \vec{\eta}^{(\alpha)}(n,t)\, \vec{\eta}^{(\alpha')}(n',t') \right\rangle$$

$$\left\langle \tilde{\eta}^{(\alpha)}(m,t)\, \tilde{\eta}^{(\alpha')}(m',t') \right\rangle = \left(\frac{2}{N}\right)^2 \int_0^N dn\, \cos\left(\frac{m\pi n}{N}\right) \int_0^N dn'\, \cos\left(\frac{m'\pi n'}{N}\right) \cdot \delta_{\alpha,\alpha'}\, \delta(n-n')\, 2D\,\delta(t-t')$$

$$= \delta_{\alpha,\alpha'} \left(\frac{2}{N}\right) \cdot 2D\, \delta(t-t') \frac{2}{N} \int_0^N dn\, \cos\left(\frac{m\pi n}{N}\right) \cos\left(\frac{m'\pi n}{N}\right).$$

$$= \frac{4D}{N}\, \delta_{\alpha,\alpha'}\, \delta_{m,m'}\, \delta(t-t').$$

- $$\tilde{\gamma}(m,t) = \tilde{\gamma}(m,0)\, e^{-\nu_m t} + \int_0^t e^{-\nu_m (t-t')}\, \tilde{\eta}(m,t')\, dt'$$

CORRELATION FUNCTIONS:

- $$\left\langle \left[\gamma^{(\alpha)}(n,t) - R_{CM}^{(\alpha)}(t)\right] \cdot \left[\gamma^{(\alpha')}(n',t') - R_{CM}^{(\alpha')}(t')\right] \right\rangle \equiv$$

$$C^{(t)}_{\alpha,\alpha'}(n,n',t,t') = \sum_{m=1}^{\infty} \sum_{m'=1}^{\infty} \cos\left(\frac{m\pi n}{N}\right) \cos\left(\frac{m'\pi n'}{N}\right) \left\langle \tilde{\gamma}^{(\alpha)}(m,t)\, \tilde{\gamma}^{(\alpha')}(m',t) \right\rangle$$

- $$\left\langle \tilde{\gamma}^{(\alpha)}(m,t)\, \tilde{\gamma}^{(\alpha')}(m',t') \right\rangle = \tilde{\gamma}^{(\alpha)}(m,0)\, e^{-\nu_m t}\, \tilde{\gamma}^{(\alpha')}(m',0)\, e^{-\nu_{m'} t'}$$

$$+ \int_0^t dt_1 \int_0^{t'} dt_2\, e^{-\nu_m (t-t_1)}\, e^{-\nu_{m'}(t'-t_2)} \underbrace{\left\langle \tilde{\eta}^{(\alpha)}(m,t_1)\, \tilde{\eta}^{(\alpha')}(m',t_2) \right\rangle}_{\displaystyle \frac{4D}{N}\, \delta_{\alpha,\alpha'}\, \delta_{m,m'}\, \delta(t_1-t_2).}$$

LONG TIME LIMIT: (STATIONARY CORRELATOR)

$$t \to \infty, \; t' \to \infty \qquad |t'-t| = \tau \text{ finite.}$$

$$\left\langle \tilde{\gamma}^{(\alpha)}(m,t)\, \tilde{\gamma}^{(\alpha')}(m',t+\tau) \right\rangle \xrightarrow{t\to\infty} \tilde{C}_{\alpha,\alpha'}(m,m',\tau)$$

$$= \lim_{t\to\infty} \int_0^t dt_1 \int_0^{t+\tau} dt_2 \; \frac{4D}{N} \delta_{\alpha,\alpha'} \delta_{m,m'} \; \delta(t_1-t_2) \,.\, e^{-\nu_m [2t+\tau-t_1-t_2]}$$

$$= \left[\lim_{t\to\infty} \underbrace{\int_0^t dt_1 \; e^{-\nu_m [2t - \cancel{2t_1}]}}_{} \right] \cdot \left[\frac{4D}{N} \delta_{\alpha,\alpha'} \delta_{m,m'} e^{-\nu_m \tau} \right]$$

$$t - t_1 = t_2$$

$$\int_0^\infty e^{-2\nu_m t_2} dt_2 = \frac{1}{2\nu_m}$$

$$\nu_m = m^2/\tau_0$$

$$\tau_0 = \frac{N^2 \gamma}{\pi^2 \lambda}.$$

$$\Rightarrow \tilde{C}_{\alpha,\alpha'}(m,m',t) = \delta_{\alpha,\alpha'} \delta_{m,m'} \cdot \frac{2D}{N} \cdot \frac{e^{-\nu_m \tau}}{\nu_m}$$

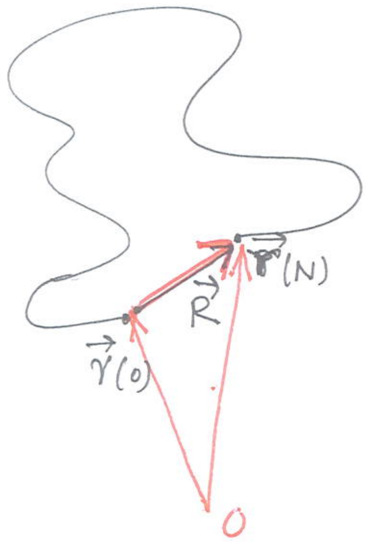
$$= \delta_{\alpha,\alpha'} \delta_{m,m'} \frac{2D\tau_0}{N} \frac{e^{-m^2(\tau/\tau_0)}}{m^2}$$

τ_0 is THE RELAXATION TIME FOR $m=1$ mode.

$$C^{(t)}_{\alpha,\alpha'}(n,n',t,t+\tau) \xrightarrow{t\to\infty} C_{\alpha,\alpha'}(n,n',\tau)$$

$$\boxed{C_{\alpha,\alpha'}(n,n',\tau) = \delta_{\alpha,\alpha'}\,\frac{2D\tau_0}{N}\sum_{m=1}^{\infty}\frac{e^{-m^2(\tau/\tau_0)}}{m^2}\cdot\cos\left(\frac{m\pi n}{N}\right)\cos\left(\frac{m\pi n'}{N}\right)}$$

END-TO-END VECTOR OF THE POLYMER:



$$\vec{R}(t) = \vec{r}(N,t) - \vec{r}(0,t).$$

$$= \Big[\underbrace{\vec{r}(N,t) - \vec{R}_{CM}(t)}_{\vec{S}_N}\Big] - \Big[\underbrace{\vec{r}(0,t) - \vec{R}_{CM}(t)}_{\vec{S}_0}\Big]$$

$$\vec{R}\cdot\vec{R} = R^2.$$

$$P(\vec{R}) = ? \quad \text{at } t\to\infty.$$

$\cancel{\langle R^2\rangle}$ $[\alpha,\alpha' \equiv x,y,z]$, $\tau = 0$

$$\langle R^{(\alpha)} R^{(\alpha')}\rangle = \left\langle \left[S_N^{(\alpha)} - S_0^{(\alpha)}\right]\left[S_N^{(\alpha')} - S_0^{(\alpha')}\right]\right\rangle$$

$$= \langle S_N^{(\alpha)} S_N^{(\alpha')}\rangle + \langle S_0^{(\alpha)} S_0^{(\alpha')}\rangle - \langle S_N^{(\alpha)} S_0^{(\alpha')}\rangle - \langle S_0^{(\alpha)} S_N^{(\alpha')}\rangle$$

$$= \delta_{\alpha,\alpha'}\,\frac{2D\tau_0}{N}\sum_{m=1}^{\infty}\frac{1}{m^2}\left[1+1-(-1)^m-(-1)^m\right]$$

$$= \delta_{\alpha,\alpha'}\,\frac{8D\tau_0}{N}\sum_{m=1}^{\infty}\frac{1}{m^2}\left[\frac{1-(-1)^m}{2}\right] \quad \leftarrow \text{sum over odd } m\text{'s.}$$

$$\frac{1-(-1)^m}{2} = 1 - \left[\frac{1+(-1)^m}{2}\right]$$

$$\left\langle R^{(\alpha)} R^{(\alpha')} \right\rangle = \delta_{\alpha,\alpha'} \frac{8D\tau_0}{N} \left[\sum_{m=1}^{\infty} \frac{1}{m^2} - \sum_{m=1}^{\infty} \frac{1}{(2m)^2} \right]$$

$$= \delta_{\alpha,\alpha'} \frac{8D\tau_0}{N} \cdot \frac{3}{4} \underbrace{\left[\sum_{m=1}^{\infty} \frac{1}{m^2} \right]}_{\zeta(2) = \frac{\pi^2}{6}}$$

$$= \delta_{\alpha,\alpha'} \frac{D\pi^2}{N} \cdot \frac{N^2\gamma}{\pi^2\lambda} .$$

$$\left\langle R^{(\alpha)} R^{(\alpha')} \right\rangle = \delta_{\alpha,\alpha'} \left(\frac{\gamma D}{\lambda}\right) N$$

$$= \delta_{\alpha,\alpha'} \frac{Na^2}{3}$$

$$\begin{cases} \lambda = \dfrac{3k_BT}{a^2} \\ \gamma D = k_BT \end{cases}$$

DISTRIBUTION :

$$\boxed{P_{ss}(\vec{R}) = \left(\frac{3}{2\pi N a^2}\right)^{3/2} \exp\left[-\frac{3R^2}{2Na^2}\right]}$$

EQUILIBRIUM MEASURE OF ROUSE CHAIN:

$$U(\{r_i\}) = \frac{\lambda}{2} \sum_{n=2}^{N} \left[(x_n - x_{n-1})^2 + (y_n - y_{n-1})^2 + (z_n - z_{n-1})^2 \right]$$

$r_i = (x_i, y_i, z_i)$, $\lambda = \frac{3k_BT}{a^2}$

At EQUILIBRIUM:

$$P[\{r_i\}] \propto e^{-\frac{U(\{r_i\})}{k_BT}}$$

For large N: $x_n - x_{n-1} \longrightarrow \frac{\partial x_n}{\partial n}$, $\sum_n^N \rightarrow \int_0^N dn$

$$P[\{r_i\}] \propto \exp\left[-\frac{3}{2b^2} \int_0^N dn \left[\left(\frac{\partial x_n}{\partial n}\right)^2 + \left(\frac{\partial y_n}{\partial n}\right)^2 + \left(\frac{\partial z_n}{\partial n}\right)^2 \right] \right]$$

MEASURE FOR A ~~3D~~ BROWNIAN MOTION TRAJECTORY/PATH IN 3-DIMENSIONS.

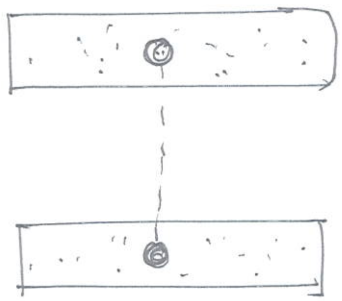
$(N \leftrightarrow t \; , \; n \leftrightarrow \tau \; , \; 2D \leftrightarrow b^2/3)$

"EACH EQUALIBRIUM POLYMER CONFIGURATION IS EQUIVALENT OF A BROWNIAN TRAJECTORY."

WHAT ABOUT A POLYMER IN EXTERNAL POTENTIAL?

ENERGY FLOW OF A BROWNIAN PARTICLE, COUPLED TO TWO HEAT BATHS AT DIFFERENT TEMPERATURES:

[Visco, JSTAT 2006]



$$T_1 \neq T_2$$

$$\boxed{m \frac{dv}{dt} = -(\gamma_1+\gamma_2)\, v + \eta_1(t) + \eta_2(t)\,.}$$

$$\langle \eta_i(t)\, \eta_j(t') \rangle = \delta_{ij}\, 2B_i\, \delta(t-t') \quad , \quad B_i = \gamma_i k_B T_i$$

Energy flow from ith bath to the particle over time t:

$$Q_i = \int_0^t d\tau\, v(\tau)\, [\eta_i - \gamma_i v]$$

Random variable. What is the distribution?

Let $i=1$ and.

$$Q_1 = \int_0^t d\tau\, v(\tau)\, [\eta_1 - \gamma_1 v] \quad : \quad P(Q, v, t)$$

$$\begin{aligned} \frac{\partial P}{\partial t} = & -\frac{\partial}{\partial v}\left[\frac{\langle \Delta v\rangle}{\Delta t} P\right] - \frac{\partial}{\partial Q_1}\left[\frac{\langle \Delta Q_1\rangle}{\Delta t} P\right] \\ & + \frac{1}{2}\frac{\partial^2}{\partial v^2}\left[\frac{\langle (\Delta v)^2\rangle}{\Delta t} P\right] + \frac{\partial^2}{\partial v\, \partial Q_1}\left[\frac{\langle \Delta v\, \Delta Q_1\rangle}{\Delta t} P\right] \\ & + \frac{1}{2}\frac{\partial^2}{\partial Q_1^2}\left[\frac{\langle (\Delta Q_1)^2\rangle}{\Delta t} P\right] \quad , \quad \Delta t \to 0\,. \end{aligned}$$

DISCRETIZATION: [also $m=1$, $(\gamma_1+\gamma_2)=\gamma$]

$$\boxed{\frac{\Delta V}{\Delta t} = -\gamma V(t) + \eta_1^{(\Delta t)}(t) + \eta_2^{(\Delta t)}(t)}$$

$$\left\langle \eta_i^{(\Delta t)}(t)\, \eta_j^{(\Delta t)}(t') \right\rangle = \begin{cases} \delta_{ij} \dfrac{2B_i}{\Delta t} & \text{as } \Delta t \to 0,\ t = t' \\ 0 & \text{for } t \neq t' \end{cases}$$

$\eta \sim \frac{1}{\sqrt{\Delta t}}$

$$\Delta Q = \Delta E = \frac{1}{2}\left[V^2(t+\Delta t) - V^2(t)\right]$$

$$= \frac{[V(t+\Delta t) + V(t)]}{2} \, \frac{[V(t+\Delta t) - V(t)]}{\Delta t} \Delta t.$$

$$= \left[V(t) + \frac{\Delta V}{2}\right]\left[-(\gamma_1+\gamma_2)V + \eta_1^{(\Delta t)} + \eta_2^{(\Delta t)}\right]\Delta t$$

$$= \left[V(t) + \frac{\Delta V}{2}\right]\left[\left(-\gamma_1 V + \eta_1^{(\Delta t)}\right) + \left(-\gamma_2 V + \eta_2^{(\Delta t)}\right)\right]\Delta t$$

$$= \Delta Q_1 \cancel{\Delta t} + \Delta Q_2 \cancel{\Delta t}.$$

$$\Rightarrow \boxed{\Delta Q_1 = \left[V(t) + \frac{\Delta V}{2}\right]\left[-\gamma_1 V + \eta_1^{(\Delta t)}\right]\Delta t}$$

$$\Delta Q_1 = \left[V(t) + \frac{\Delta V}{2}\right](-\gamma_1 V)\Delta t + \left[V(t) + \frac{\Delta V}{2}\right]\eta_1^{(\Delta t)}(t)\, \Delta t.$$

$\lim \Delta t \to 0$

$$\frac{\langle \Delta v \rangle}{\Delta t} = -\gamma v \quad , \quad \cancel{\frac{\langle \Delta Q \rangle}{\Delta t}} =$$

$$\frac{\langle \Delta v^2 \rangle}{\Delta t} = 2(B_1 + B_2) \equiv 2B$$

$\langle \Delta v \rangle \sim \Delta t + \sqrt{\Delta t}$

$\langle (\Delta v)^2 \rangle \sim \Delta t \cdot \cdot$

$$\left\langle \Delta v \, \eta_1^{(\Delta t)} \right\rangle = \Delta t \left\langle \left(\eta_1^{(\Delta t)}\right)^2 \right\rangle = 2B_1$$

$\Rightarrow \cancel{\langle \Delta v \, \Delta Q_1 \rangle}$

$$\Rightarrow \frac{\langle \Delta Q_1 \rangle}{\Delta t} = -\gamma_1 v^2 + B_1$$

$$\frac{\langle \Delta v \cdot \Delta Q_1 \rangle}{\Delta t} = v \cdot \Delta t \left\langle \left(\eta_1^{\Delta t}\right)^2 \right\rangle = v \cdot 2B_1 .$$

$$\frac{\langle (\Delta Q_1)^2 \rangle}{\Delta t} = v^2 \left\langle \left(\eta_1^{(\Delta t)}\right)^2 \right\rangle \Delta t = v^2 \, 2B_1$$

FP EQUATION:

$$\boxed{\begin{aligned} \frac{\partial P}{\partial t} &= +\gamma \frac{\partial}{\partial v}\left[v P\right] + \left(\gamma_1 v^2 - B_1\right) \frac{\partial P}{\partial Q_1} \\ &\quad + B \frac{\partial^2 P}{\partial v^2} + 2B \frac{\partial}{\partial v}\left[v \frac{\partial P}{\partial Q_1}\right] + B_1 v^2 \frac{\partial^2 P}{\partial Q_1^2} \end{aligned}}$$

Define:

$$\rho_\lambda(v,t) = \int_{-\infty}^{+\infty} e^{-\lambda Q_1} P(Q_1, v, t)\, dQ_1 \qquad (\lambda = ik).$$

(Fourier Transform).

Then:

$$P(Q_1, v, t) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} \rho_\lambda(v,t)\, e^{\lambda Q}\, d\lambda .$$

$$\rightarrow \int_{-\infty}^{+\infty} dQ_1\, e^{-\lambda Q_1} \Big[\text{FP Eqn of } P(Q_1, v, t) \Big]$$

$$\cdot \int_{-\infty}^{+\infty} dQ_1\, e^{-\lambda Q_1} \frac{\partial P}{\partial Q_1} = \cancel{e^{-\lambda Q_1} P(Q_1, v, t) \Big|_{-\infty}^{+\infty}}^{\,0} + \lambda \int_{-\infty}^{+\infty} e^{-\lambda Q_1} P(Q_1, v, t)\, dQ_1$$

$$= \lambda\, \rho_\lambda(v,t)$$

$$\cdot \int_{-\infty}^{+\infty} dQ_1\, e^{-\lambda Q_1} \frac{\partial^2 P}{\partial Q_1^2} = \lambda^2 \rho_\lambda(v,t) .$$

FP EQ. FOR ρ_λ:

$$\boxed{\begin{aligned} \frac{\partial \rho_\lambda}{\partial t} &= B \frac{\partial^2 \rho_\lambda}{\partial v^2} + (\gamma + 2\lambda B_1) \frac{\partial}{\partial v}\left[v \rho_\lambda \right] \\ &\quad + \left[(B_1 \lambda^2 + \gamma_1 \lambda) v^2 - B_1 \lambda \right] \rho_\lambda(v,t) \end{aligned}}$$

$\lambda = 0$: $\quad \dfrac{\partial \rho_0}{\partial t} = B \dfrac{\partial^2 \rho_0}{\partial v^2} + \gamma \dfrac{\partial}{\partial v}\left[v \rho_0 \right] \longrightarrow$ OU PROCESS.

$g_\lambda(v,t|v_0)$ in terms of the Quantum problem:

$$U(v) = \frac{v^2}{2}$$

[$\gamma \to (\gamma + 2\lambda B_1)^{-1}$, $D \to B$ in the earlier problem.]

$$\Rightarrow \quad g_\lambda(v,t|v_0) = e^{-\left(\frac{\gamma+2\lambda B_1}{4B}\right)[v^2 - v_0^2]} \langle v | e^{-Ht} | v_0 \rangle$$

- $$H = -B\frac{\partial^2}{\partial v^2} + W(v) \qquad \left[\frac{\hbar^2}{2} = B \right]$$

Look at the eqn.

- $$W(v) = \frac{(\gamma+2\lambda B_1)^2}{4B} v^2 - \frac{(\gamma+2\lambda B_1)}{2}$$ [From transformation of the potential]

$$- \left[+ (B_1\lambda^2 + \gamma_1\lambda) v^2 - B_1\lambda . \right]$$ [from the extra term in FP eqn.]

$$= \frac{1}{2}\omega^2 v^2 - \Delta E \ , \qquad \Delta E = \frac{\gamma}{2} + \ldots$$

$$\omega^2 = \frac{1}{2B}\left[(\gamma + 2\lambda B_1)^2 \cancel{+} 4\underset{\downarrow (B_1+B_2)}{B} (B_1\lambda^2 + \gamma_1\lambda) \right]$$

or, $$(\hbar\omega)^2 = \left[\gamma^2 + 4\lambda^2 B_1^2 + 4\underset{\hookrightarrow(\gamma_1+\gamma_2)}{\gamma}\lambda B_1 \cancel{+} 4(B_1+B_2)(B_1\lambda^2 + \gamma_1\lambda) \right]$$

$$= \gamma^2 \left[1 + \frac{4\lambda}{\gamma^2}(\gamma_2 B_1 - \gamma_1 B_2 - \lambda B_1 B_2) \right]$$

[Check].

- $\hbar\omega = \gamma\mu(\lambda)$
- $$\frac{\hbar}{\omega} = \frac{\hbar^2}{\hbar\omega} = \frac{2B}{\gamma\mu}$$

$\frac{B}{\gamma} = T_0$ $\quad T^* = T_0/\mu$ $\quad = 2T^*$

- $$\mu(\lambda) = \left[1 + \frac{4\lambda}{\gamma^2} \underbrace{(\gamma_2 B_1 - \gamma_1 B_2 - \lambda B_1 B_2)}_{\substack{\parallel \\ B_1 B_2(\Delta\beta - \lambda)}} \right]^{1/2}$$

- $$\Delta\beta = \frac{1}{k_B}\left[\frac{1}{T_2} - \frac{1}{T_1} \right] ,$$

$$\langle v | e^{-Ht} | v_0 \rangle = \sum_{n=0}^{\infty} e^{-E_n t}\, \psi_n(v)\, \psi_n(v_0)$$

$$E_n = \hbar\omega\,(n+1/2) - \Delta E = \frac{\gamma}{2}\left[(2n+1)\mu - 1 \right]$$

$$\psi_n(v) = \frac{1}{\sqrt{2^n n!}} \left(\frac{\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{\omega}{2\hbar} v^2} H_n\!\left(\sqrt{\frac{\omega}{\hbar}}\, v\right)$$

$$= \frac{1}{\sqrt{2^n n!}} \left(\frac{1}{2\pi T^*}\right)^{1/4} e^{-\frac{v^2}{4T^*}} H_n\!\left(\frac{v}{\sqrt{2T^*}}\right)$$

$$\boxed{\rho_\lambda(v,t|v_0) = e^{-\left(\frac{\gamma + 2\lambda B_1}{4B}\right)(v^2 - v_0^2)} \cdot \frac{e^{-\frac{1}{4T^*}(v^2+v_0^2)}}{\sqrt{2\pi T^*}} \sum_{n=0}^{\infty} \frac{e^{-E_n t}}{2^n n!} H_n\!\left(\frac{v}{\sqrt{2T^*}}\right) H_n\!\left(\frac{v_0}{\sqrt{2T^*}}\right)}$$

LARGE t Limit:

$$\rho_\lambda(v,t|v_0) \approx e^{-\frac{\gamma}{2}(\mu(\lambda)-1)t} \cdot e^{-\frac{1}{2}\left(\frac{\gamma+2\lambda B_1}{2B} + \frac{1}{2T^*}\right)v^2} \cdot \frac{e^{-\frac{1}{2}\left(-\frac{\gamma+2\lambda B_1}{2B} + \frac{1}{2T^*}\right)v_0^2}}{\sqrt{2\pi T^*}}$$

$$\mu(0) = 1, \quad T^*(0) = \frac{B}{\gamma} = T_0$$

$$\rho_0(v,t|v_0) \approx \frac{e^{-\frac{1}{2}\frac{v^2}{T_0}}}{\sqrt{2\pi T_0}}$$

← steady state ~~equilibrium~~ distribution.

- Integrating the final velocity, and averaging over the initial velocity with respect to the stationary distribution:

$$\tilde{P}(\lambda,t) = \int_{-\infty}^{+\infty} dv \cdot \int_{-\infty}^{+\infty} dv_0 \cdot \frac{e^{-\frac{v_0^2}{2T_0}}}{\sqrt{2\pi T_0}} \, \rho_\lambda(v,t|v_0) .$$

or, $$\boxed{\tilde{P}(\lambda,t) = g(\lambda)\, e^{-\nu(\lambda)t}} \quad , \quad \nu(\lambda) = \frac{\gamma}{2}\left[-1+\mu(\lambda)\right]$$

$$g(\lambda) = \frac{1}{\sqrt{T^* T_0}} \cdot \left[\frac{1}{2T^*} + \frac{\gamma+2\lambda B_1}{2B}\right]^{-1/2} \left[\frac{1}{2T^*} + \frac{1}{T_0} - \frac{\gamma+2\lambda B_1}{2B}\right]^{-1/2}$$

$T^* = \frac{T_0}{\mu}$

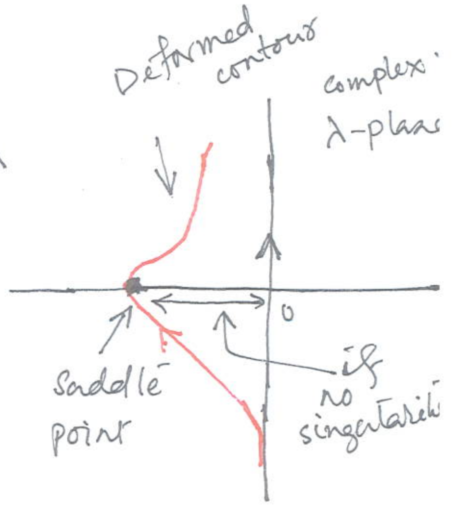
$T_0 = \frac{B}{\gamma}$

$$= \frac{\mu^{1/2}}{T_0}\left[\frac{\mu}{2T_0} + \frac{\gamma+2\lambda B_1}{2B}\right]^{-1/2}\left[\frac{\mu}{2T_0} + \frac{1}{T_0} - \frac{\gamma+2\lambda B_1}{2B}\right]^{-1/2}$$

$$= \mu^{1/2}\, 2\left[\mu + \frac{\gamma+2\lambda B_1}{\gamma}\right]^{-1/2}\left[\mu + 2 - \frac{\gamma+2\lambda B_1}{\gamma}\right]^{-1/2}$$

$$= 2\gamma\sqrt{\mu}\left[\gamma(1+\mu) + 2\lambda B_1\right]^{-1/2}\left[\gamma(1+\mu) - 2\lambda B_1\right]^{-1/2}$$

$$P(Q_1,t) = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} g(\lambda)\, e^{\nu(\lambda)t}\, e^{\lambda Q_1}\, d\lambda$$

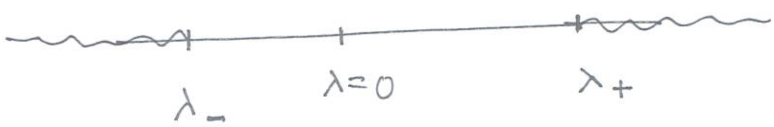


SINGULARITIES OF $\mu(\lambda)$: [Branch points]

$$4B_1B_2\lambda^2 - 4(\gamma_2B_1-\gamma_1B_2)\lambda - \gamma^2 = 0$$

$$\lambda_\pm = \frac{(\gamma_2B_1-\gamma_1B_2) \pm \sqrt{(\gamma_2B_1-\gamma_1B_2)^2+\gamma^2B_1B_2}}{2B_1B_2}$$

$$\gamma_2B_1-\gamma_1B_2 = \underline{\gamma_1\gamma_2}\, k_B[T_1-T_2]$$



SINGULARITIES OF $g(\lambda)$:

$$\boxed{\gamma\mu + (\gamma \pm 2\lambda B_1) = 0}\ , \quad \lambda \neq 0$$

$$\gamma\mu = -(\gamma \pm 2\lambda B_1)$$

$$\Rightarrow (\gamma\mu)^2 = \gamma^2 \pm 4\lambda\gamma B_1 + 4\lambda^2B_1^2.$$

$$\Rightarrow \cancel{\gamma^2} + 4\lambda(\gamma_2B_1-\gamma_1B_2) - 4\lambda^2B_1B_2 = \cancel{\gamma^2} \pm 4\lambda\gamma B_1 + 4\lambda^2B_1^2$$

$$\Rightarrow \lambda\left[\lambda(\underbrace{B_1^2+B_1B_2}_{B_1B}) - (\gamma_2B_1-\gamma_1B_2 \mp \gamma B_1)\right] = 0$$

SINGULARITIES OF $g(\lambda)$:

$$\lambda^*_{\pm} = \frac{(\gamma_2 B_1 - \gamma_1 B_2) \pm \gamma B_1}{B_1 B}. \qquad B = B_1 + B_2$$

$$\lambda^*_{-} = \frac{\cancel{\gamma_2 B_1} - \gamma_1 B_2 - (\gamma_1 + \cancel{\gamma_2}) B_1}{B_1 B}$$

$$= - \frac{\gamma_1 (\cancel{B_1 + B_2})}{B_1 \cancel{B}} \Rightarrow \boxed{\lambda^*_{-} = - \frac{\gamma_1}{B_1} = - \frac{1}{k_B T_1}}$$

$$\lambda^*_{+} = \frac{\gamma_2 B_1 - \gamma_1 B_2 + (\gamma_1 + \gamma_2) B_1}{B_1 B}$$

$$= \frac{\gamma_2 B_1 - \gamma_1 (B - B_1) + (\gamma_1 + \gamma_2) B_1}{B_1 B}$$

$$= \frac{B_1 [\gamma_2 + \gamma_1 + \gamma_1 + \gamma_2] - \gamma_1 B}{B_1 B}$$

$$\boxed{\lambda^*_{+} = \frac{2\gamma}{B} - \frac{\gamma_1}{B_1}}$$

$$\lambda^*_{+} = \frac{(\gamma_2 B_1 - \gamma_1 B_2)}{B_1 B} + \frac{\gamma}{B}.$$

- If $\lambda^*_\pm$ is outside the range $[\lambda_-, \lambda_+]$:

Then one does not have to worry about the prefactor $g(\lambda)$ in the saddle point calculation:

$$P(Q,t) \approx \frac{1}{2\pi i}\int_{-i\infty}^{+i\infty} d\lambda\, e^{-t\left[\nu(\lambda) - \lambda \frac{Q}{t}\right]} \sim e^{-t\,\Phi(Q/t)}$$

~~where $\Phi(q) = \min[$~~

where, $\Phi(q) = \nu(\lambda^*) - \lambda^* q$.

and λ^* is the solution of $\nu'(\lambda^*) = q$

FINDING THE SADDLE POINT:

$$\nu(\lambda) = \frac{\gamma}{2}(\mu - 1)$$

$$\nu(\lambda^*) = \frac{\gamma}{2}\left[\mu(\lambda^*) - 1\right]$$

$$\nu'(\lambda) = q$$

$$\Rightarrow \boxed{\frac{\gamma}{2}\mu'(\lambda) = q}$$

$$\mu(\lambda) = \frac{2\sqrt{B_1 B_2}}{\gamma}\sqrt{(\lambda_+ - \lambda)(\lambda - \lambda_-)}, \quad \lambda_- < \lambda < \lambda_+$$

Differentiating:

$$\Rightarrow \frac{\sqrt{B_1 B_2}}{2\mu(\lambda^*)}\Big[\underbrace{(\lambda_+ + \lambda_-) - 2\lambda^*}_{(\lambda_+ - \lambda^*) - (\lambda^* - \lambda_-)}\Big] = q, \text{ for given } q.$$

$\lambda^* \to \lambda_+ \;:\; q \to -\infty$

$\lambda^* \to \lambda_- \;:\; q \to +\infty$

$$\boxed{(\lambda_+ + \lambda_-) - 2\lambda^* = \frac{2q}{\sqrt{B_1 B_2}}\,\mu(\lambda^*)}$$

$$\begin{cases} \alpha_1 = \lambda_+ + \lambda_- \\ q_0 = \frac{2q}{\sqrt{B_1 B_2}} \\ \alpha_2 = \lambda_+ \lambda_- \end{cases}$$

Squaring both sides:

$$\alpha_1^2 + 4\lambda^{*2} - 4\alpha_1\lambda^* = q_0^2 \mu^2$$

$$= q_0^2 \left[-\alpha_2 + \alpha_1\lambda^* - \lambda^{*2} \right]$$

$$\Rightarrow (4 + q_0^2)\lambda^{*2} - (4\alpha_1 + \alpha_1 q_0^2)\lambda^* + \alpha_1^2 + \alpha_2 q_0^2 = 0.$$

$$\Rightarrow \lambda^{*2} - \alpha_1\lambda^* + \frac{\alpha_1^2 + \alpha_2 q_0^2}{4 + q_0^2} = 0.$$

$$\lambda^* = \frac{\alpha_1}{2} \pm \frac{1}{2}\Big[\underbrace{\alpha_1^2 - 4\left(\frac{\alpha_1^2 + \alpha_2 q_0^2}{4 + q_0^2}\right)}\Big]^{1/2}$$

$$\frac{\cancel{4\alpha_1^2} + \alpha_1^2 q_0^2 - \cancel{4\alpha_1^2} - 4\alpha_2 q_0^2}{4 + q_0^2}$$

$$= \frac{q_0^2(\alpha_1^2 - 4\alpha_2)}{4 + q_0^2} = \frac{q_0^2(\lambda_+ - \lambda_-)^2}{4 + q_0^2}$$

$$= \frac{\lambda_+ + \lambda_-}{2} \pm \frac{|q|(\lambda_+ - \lambda_-)}{2\sqrt{q^2 + B_1 B_2}}$$

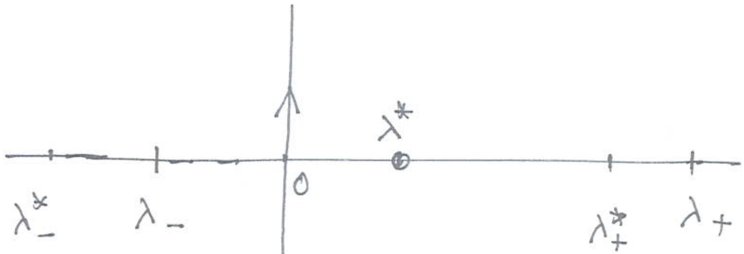
$$\rightarrow = \frac{\lambda_+ + \lambda_-}{2} - \frac{q}{\sqrt{B_1 B_2}}\mu(\lambda^*)$$

$$\mu(\lambda^*) > 0$$

$$\Rightarrow \boxed{\lambda^*(q) = \frac{\lambda_+ + \lambda_-}{2} - \frac{q(\lambda_+ - \lambda_-)}{2\sqrt{q^2 + B_1 B_2}}}$$

$$\boxed{\mu(\lambda^*) = \frac{\sqrt{B_1 B_2}(\lambda_+ - \lambda_-)}{2\sqrt{q^2 + B_1 B_2}}}$$

The above saddle-point calculation works as long as:

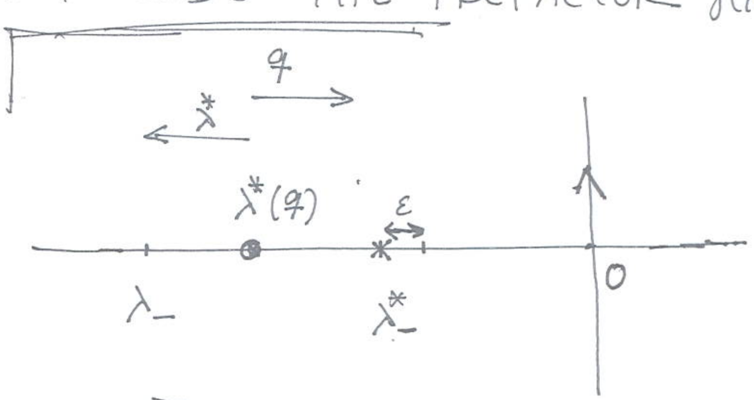


~~Mine~~

$$\boxed{\mathrm{Max}(\lambda^*_-, \lambda_-) < \lambda^* < \mathrm{Min}(\lambda^*_+, \lambda_+)}$$

OTHERWISE ONE NEEDS TO INCLUDE THE PREFACTOR $g(\lambda)$ IN THE CALCULATION.

FOR EXAMPLE, SUPPOSE:



$$\Phi(q) = \min_\lambda \Big[\underbrace{\nu(\lambda) - \lambda q - \frac{1}{t}\ln g(\lambda)}_{= f}\Big]$$

$\underline{g(\lambda^*_-) = \infty :}$ $\quad \Rightarrow \quad g(\lambda) \sim \dfrac{\text{const.}}{\varepsilon^\alpha}, \quad \lambda = \lambda^*_+ + \varepsilon \quad \text{as } \varepsilon \to 0$, $\quad \alpha > 0$

$$f(\varepsilon) \approx \nu(\lambda^*_-) + \varepsilon \nu'(\lambda^*_-) - \lambda^*_- q - \varepsilon q + \frac{\alpha}{t}\ln \varepsilon + \text{const.}$$

$$f'(\varepsilon) = 0 \Rightarrow \varepsilon = \frac{\alpha}{t} \cdot \frac{1}{q - \nu'(\lambda^*_-)}$$

$$\Rightarrow f(\varepsilon) \simeq [\text{const.}] - \lambda^*_- q + O\left(\frac{1}{t}\right) + O\left(\frac{1}{t}\ln t\right)$$

$$\Rightarrow \Phi(q) \xrightarrow{t \to \infty} -\lambda^*_- q + [\text{const}]$$

$$\underline{Q = qt}$$

- $P(Q) \sim e^{\lambda_-^* Q}$ [Note $\lambda_-^* = -\frac{1}{k_B T_1} < 0$

for $q > q_-^*$. ~~where $\lambda^*(q) = \lambda^*$~~

where q_-^* is given by $\boxed{\lambda^*(q_-^*) = \lambda_-^*}$

similarly

- $P(Q) \sim e^{\lambda_+^* Q}$ for $q < q_+^*$

given by $\lambda^*(q_+^*) = \lambda_+^*$

THE ORIGIN OF SINGULARITIES IN $g(\lambda)$:

$$\tilde{P}(\lambda,t) = \int_{-\infty}^{+\infty} e^{-\lambda Q} P(Q,t)\, dt \sim g(\lambda)\, e^{\nu(\lambda) t}.$$

- If $P(Q,t)$ decays faster than exponentially, the integral converges for all λ.
- If $P(Q,t)$ decays slower than exponential tail, the integral diverges for all λ.
- Iff $P(Q,t)$ has exponential tail, say $P(Q) \sim e^{-aQ}$, as $Q \to \infty$, then $\tilde{P}(\lambda,t)$ has a singularity at $\lambda = -a$.

$\lambda \le -a$: the integral diverges.

The symmetry $\mu(\lambda) = \mu(\Delta\beta - \lambda)$:

$\hookrightarrow \quad \nu(\lambda) = \nu(\Delta\beta - \lambda)$.

$$P(Q) \approx \int e^{\nu(\lambda)} e^{\lambda Q} \, d\lambda$$

$$= \int e^{\nu(\Delta\beta - \lambda)} e^{\lambda Q} \, d\lambda \qquad \Delta\beta - \lambda = \lambda'$$

$$= \int e^{\nu(\lambda')} e^{(\Delta\beta - \lambda')Q} \, d\lambda'$$

$$= e^{\Delta\beta Q} \underbrace{\int e^{\nu(\lambda')} e^{\lambda'(-Q)} \, d\lambda'}_{P(-Q)}$$

$$\Rightarrow \boxed{\frac{P(Q)}{P(-Q)} = e^{\Delta\beta Q}}$$

$$P(Q) \sim e^{-t\,\Phi(Q/t)}$$

$$\Rightarrow \boxed{\Phi(q) - \Phi(-q) = -\Delta\beta q}$$