Chapter 1 Classical theory (Wiener path integrals)

1.1 Brownian motion

- Macroscopic derivation of diffusion eq. (1D)

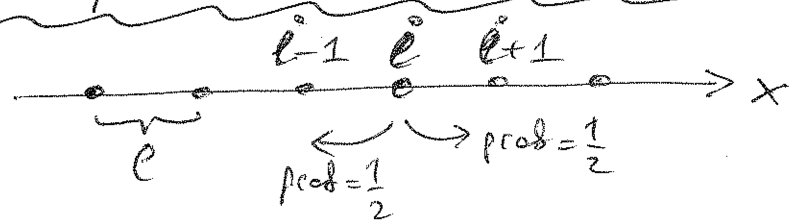
$$\cancel{j = -D\frac{\partial\rho(x,t)}{\partial x} = \frac{dN}{dt\,\Delta S}}, \quad \cancel{\frac{dN}{dt} \overset{\text{also}}{=} \frac{\partial\rho(x,t)}{\partial t}\Delta V = -\frac{\partial j(x,t)}{\partial x}\Delta S}$$

$$dN \cancel{= [\rho(x+dx,t) - \rho(x,t)]}$$

Continuity eq-n 1D: $\frac{\partial j}{\partial x} + \frac{\partial \rho}{\partial t} = 0$

$$j = -D\frac{\partial\rho}{\partial x} \Rightarrow \boxed{\frac{\partial\rho}{\partial t} = D\frac{\partial^2\rho}{\partial x^2}}$$

- Microscopic derivation via random walk (equal right/left probabilities)



Prob. of transition over time ε:

$$W(il - jl, \varepsilon) = \begin{cases} 1/2, & \text{if } i = j+1 \text{ (to the right)} \\ 1/2, & \text{if } i = j-1 \text{ (to the left)} \\ 0, & \text{if } |i-j| > 1 \text{ (only to the nearest sites)} \end{cases}$$

Transitions are statistically independent! (Markov chain)

$W_i(t_n)$ – prob. for the site i to be occupied at t_n

$$\boxed{W_i(t_n) = \sum_j \underbrace{W_{ij}(t_n)}_{\text{transition probability}} W_j(0)}$$

$W_i(0) \in [0,1]$

$W_{ij} \in [0,1]$

$\sum_i W_i(0) = 1$

$\sum_j W_{ij} = 1, \ \forall i$

$$\boxed{\text{form matrix } W(t_n)} \leftarrow W(il - jl, \underbrace{t_n}_{n\varepsilon})$$

Since events are independent:

$$\boxed{W(il - jl, n\varepsilon) = [W(\varepsilon)]^n_{ij}} \qquad (1.1.6)$$

~~write~~ ~~write~~

since

$$W_i(\varepsilon) = \sum_{k_1} W_{ik_1}(\varepsilon)\, W_{k_1}(0)$$

$$W_i(2\varepsilon) = \sum_{k_2} W_{ik_2}(\varepsilon)\, W_{k_2}(\varepsilon) = \sum_{k_1 k_2} W_{ik_2}(\varepsilon) W_{k_2 k_1}(\varepsilon) W_{k_1}(0)$$

$$= \sum_{k_1} \left[W(\varepsilon)\right]^2_{ik_1} W_{k_1}(0) \equiv \sum_j W_{ij}(2\varepsilon)\, W_j(0)$$

$$\hookrightarrow W_{ij}(2\varepsilon) = \left[W(\varepsilon)\right]^2_{ij}$$

similarly for 3ε, 4ε, etc.

- At $t=0$, $x=0 \rightarrow w_i(0) = \delta_{i0}$

$$\hookrightarrow w_i(n\varepsilon) = \sum_j \left(W(\varepsilon)\right)^n_{ij} \delta_{j0} \Rightarrow \boxed{w(n\varepsilon) = W^n(\varepsilon)\, w(0)}$$

- Introduce:

$$R_{ij} = \delta_{i,j+1} \;;\; L_{ij} = \delta_{i+1,j}$$

$$w_i' \equiv \sum_j R_{ij} w_j = \sum_j \delta_{i,j+1} w_j = w_{i-1} \rightarrow$$ (the distribution w_i moves to the right)

$$w_i'' = \sum_j L_{ij} w_j = \sum_j \delta_{i+1,j} w_j = w_{i+1} \rightarrow$$ (w_i move to the left)

for instance, if $w_j = \delta_{j0} \rightarrow w_j' = \delta_{j-1,0} = \delta_{j,1}$, i.e. the occ site moved to the right; $w_j'' = \delta_{j+1,0} = \delta_{j,-1} \rightarrow$ moved indeed to the left.

Multiply:

$$RL = \sum_k R_{ik} L_{kj} = \sum_k \delta_{i,k+1}\, \delta_{k+1,j} = \delta_{ij} \equiv \mathbb{1} \rightarrow R = L^{-1},\ L = R^{-1}$$

Also,

$$\frac{1}{2}(R+L) = \frac{1}{2}\left(\delta_{i,j+1} + \delta_{i+1,j}\right) = \frac{1}{2}\left(\delta_{i,j+1} + \delta_{i,j-1}\right)$$

which is the same as W_{ij}, i.e., $\boxed{W = \frac{1}{2}(R+L)}$

- We have to calculate $[W(\varepsilon)]^n$:

$$W^n = \left[\frac{1}{2}(R+L)\right]^n = \frac{1}{2^n} \sum_{k=0}^{n} \binom{n}{k} R^k L^{n-k}$$

$$= \frac{1}{2^n}\sum_{k=0}^{n}\binom{n}{k}\underbrace{R^k R^{-(n-k)}}_{R^{2k-n}} \overset{\text{or}}{\equiv} \frac{1}{2^n}\sum_{k=0}^{n}\binom{n}{k}\underbrace{L^{-k}L^{n-k}}_{L^{n-2k}}$$

However,

$$(R^K)_{ij} = \delta_{i,j+k}\ , \ (L^K)_{ij} = \delta_{i+k,j}$$

---

indeed,

$$(R^2)_{ij} = \sum_k R_{ik}R_{kj} = \sum_k \delta_{i,k+1}\underbrace{\delta_{k,j+1}}_{k=j+1} = \delta_{i,j+1+1} = \delta_{i,j+2}$$

$$(R^3)_{ij} = \sum_k R_{ik}R^2_{kj} = \sum_k \delta_{i,k+1}\delta_{k,j+2} = \delta_{i,j+3}\text{, etc.}$$

- Then,

$$(W^n)_{ij} = \frac{1}{2^n}\sum_{k=0}^{n}\binom{n}{k}(R^{2k-n})_{ij} = \frac{1}{2^n}\sum_{K=0}^{n}\binom{n}{k}\delta_{i,j+2k-n}$$

$$= \frac{1}{2^n}\left[\binom{n}{0}\delta_{i,j-n} + \binom{n}{1}\delta_{i,j+2-n} + \binom{n}{2}\delta_{i,j+4-n} + \dots + \binom{n}{n}\delta_{i,j+n}\right]$$

~~Nonzero~~ $\mapsto$ $2k = i-j+n$ (should be even!)

- Non-zero element appears if $0 \le i-j+n \le 2n$, ~~or ...~~

or $-n \le i-j \le n \rightarrow \boxed{|i-j| \le n}$.

So,

$$(W^n)_{ij} \equiv W(il-jl, n\varepsilon) = \begin{cases} 0, \text{ if } |i-j|>n \text{ or } i-j+n=\text{odd} \\ \frac{1}{2^n}\binom{n}{\frac{i-j+n}{2}}, \text{ if } |i-j|\le n \text{ and } i-j+n=\text{even} \end{cases} \quad (1.1.13)$$

- Starting from the initial distribution $W_i(0) = \delta_{i0}$, we have after $t = n\varepsilon$:

$$\boxed{W_i(n\varepsilon) = \sum_j [W(\varepsilon)]^n_{ij}\delta_{j0} = [W(\varepsilon)]^n_{i0} = \begin{cases} 0, \text{ if } |i|>n \text{ or } i+n=\text{odd} \\ \frac{1}{2^n}\binom{n}{\frac{1}{2}(i+n)}, \text{ if } |i|\le n,\ i+n=\text{even}\end{cases}} \quad (1.1.14)$$

this the central result!

• Introducing space and time variables: $x = i\ell$, $t = n\varepsilon$:

$$W(i\ell, n\varepsilon) = W_i(n\varepsilon) \to W(x,t)$$

$$\underbrace{W(\underbrace{x}_{i\ell}, \underbrace{t+\varepsilon}_{(n+1)\varepsilon})} = \left\{ \begin{array}{ll} 0, & \text{if } |i| > n+1,\ i+n+1 = \text{odd} \\ \frac{1}{2^{n+1}}\binom{n+1}{\frac{1}{2}(i+n+1)}, & \text{otherwise} \end{array} \right\}.$$

$$W(\underbrace{x+\ell}_{(i+1)\ell}, \underbrace{t}_{n\varepsilon}) = \left\{ \begin{array}{ll} 0, & \text{if } |i+1| > n,\ i+1+n = \text{odd} \\ \frac{1}{2^n}\binom{n}{\frac{1}{2}(i+1+n)}, & \text{otherwise} \end{array} \right.$$

$$W(\underbrace{x-\ell}_{(i-1)\ell}, \underbrace{t}_{n\varepsilon}) = \left\{ \begin{array}{ll} 0, & \text{if } |i-1| > n,\ i-1+n = \text{odd} \\ \frac{1}{2^n}\binom{n}{\frac{1}{2}(i-1+n)}, & \text{otherwise.} \end{array} \right.$$

Consider sites $i+n+1 = \text{even}$ (also means $i-1+n = \text{even}$) and $|i| \le n+1 \to -(n+1) \le i \le n+1$, as for $W(x, t+\varepsilon)$. For these sites

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

$$= \frac{1}{2}\Big[\underbrace{\frac{1}{2^n}\binom{n}{\frac{1}{2}(i+n+1)}}_{\text{as in } W(x+\ell,t)} + \underbrace{\frac{1}{2^n}\binom{n}{\frac{1}{2}(i-1+n)}}_{\text{as in } W(x-\ell,t)}\Big]$$

~~But we need to check conditions on sites; odd/even = ok;~~

~~$W(x+\ell,t) \to |i+1| \le n \to -n \le i+1 \le n,\ -(n+1) \le i \le n-1,$~~

~~so only $i = n, n+1$ need to be checked.~~

so that we can write:

$$\boxed{W(x, t+\varepsilon) = \frac{1}{2}\left[W(x+\ell, t) + W(x-\ell, t)\right]} \qquad (1.1.15)$$

This is ok for the binomial coeff., but we need to check the conditions on sites.

$W(x+\ell,t)\neq 0 \to i+1+n=$ even, $|i+1|\le n$ or $-(n+1)\le i\le n-1$

$W(x-\ell,t)\neq 0 \to i-1+n=$ even (the same), $|i-1|\le n$, $-(n-1)\le i\le n+1$

$W(x,t+\varepsilon)\neq 0 \to i+n+1=$ even (the same), $|i|\le n+1$, $-(n+1)\le i\le n+1$

So, (1.1.15) is definitely valid for any $-(n-1)\le i\le n-1$.
We need to check sites: $i=\mp n, \mp(n+1)$.

(a) $\underline{i=n}$ $\to$ $W(x-\ell,t)=0$ as $i-1+n=2n-1=$ odd

$W(x+\ell,t)=0$

$W(x,t+\varepsilon)=0$ as well as $i+n+1=2n+1=$ odd

i.e. (1.1.15) is fullfilled.

(b) $\underline{i=n+1}$ $\to$ $W(x-\ell,t)=\frac{1}{2^n}\binom{n}{\frac{1}{2}(2n)}=\frac{1}{2^n}\binom{n}{n}=\frac{1}{2^n}$

$W(x+\ell,t)=0$ as $|i+1|=|n+2|>n$

$W(x,t+\varepsilon)=\frac{1}{2^{n+1}}\binom{n+1}{\frac{1}{2}(2n+2)}=\frac{1}{2^{n+1}}\binom{n+1}{n+1}=\frac{1}{2^{n+1}}$

i.e. (1.1.15) is ok again.

(c) $\underline{i=-n}$ $\to$ $W(x-\ell,t)=0$, $W(x+\ell,t)=0$, $W(x,t+\varepsilon)=0$
as $i+n\pm 1=-n+n\pm 1=$ odd

(d) $i=-n-1$ $\to$ $W(x-\ell,t)=0$

$W(x+\ell,t)=\frac{1}{2^n}\binom{n}{\frac{1}{2}(-n-1+1+n)}=\frac{1}{2^n}\binom{n}{0}=\frac{1}{2^n}$

$$w(x,t+\varepsilon) = \frac{1}{2^{n+1}} \begin{pmatrix} n+1 \\ \frac{1}{2}(-n-1+n+1) \end{pmatrix} = \frac{1}{2^{n+1}}$$

so that (1.1.15) is valid again.

- So, (1.1.15) is valid for <u>all</u> sites. We rewrite it:

$$\frac{w(x,t+\varepsilon)-w(x,t)}{\varepsilon} = \underbrace{\frac{1}{2}\,\frac{w(x+\ell,t)+w(x-\ell,t)}{\varepsilon} - \frac{w(x,t)}{\varepsilon}}_{\frac{1}{2}\,\frac{w(x+\ell,t)-2w(x,t)+w(x-\ell,t)}{\varepsilon}}$$

or

$$\underbrace{\frac{w(x,t+\varepsilon)-w(x,t)}{\varepsilon}}_{\partial w/\partial t} = \underbrace{\frac{\ell^2}{2\varepsilon}}_{D}\;\underbrace{\frac{w(x+\ell,t)-2w(x,t)+w(x-\ell,t)}{2\ell}}_{\partial^2 w/\partial x^2}$$

I.e. we have the diffusion eq. again.

- <u>Solution of the diffusion eq.</u>

Assume that $\boxed{w(x,t) = \delta(x) \text{ at } t=0.}$

Apply FT:

$$\frac{\partial w}{\partial t} = \mathcal{D}\frac{\partial^2 w}{\partial x^2}, \quad w(x,t) = \int dk\, e^{ikx}\, W(k,t)$$

$$\hookrightarrow \dot{W}(k,t) = \mathcal{D}(ik)^2 W(k,t) = -\mathcal{D}k^2 W(k,t)$$

$$W(k,t) = C e^{-\mathcal{D}k^2 t}$$

At $t=0 \to w(x,0) = \int dk\, e^{ikx} W(k,0) \equiv \delta(x) = \frac{1}{2\pi}\int dk\, e^{ikx}$

$\hookrightarrow W(k,0) = 1/2\pi$ and $W(k,t) = \frac{1}{2\pi} e^{-\mathcal{D}k^2 t}$

and $$W(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{-\mathcal{D}k^2 t}\, e^{ikx}$$

$$= \frac{1}{2\pi} \int dk\, \exp\left[-\mathcal{D}t\left(k^2 - 2\frac{ix}{2\mathcal{D}t}k + \left(\frac{ix}{2\mathcal{D}t}\right)^2 - \left(\frac{ix}{2\mathcal{D}t}\right)^2\right)\right]$$

$$= \frac{1}{2\pi} \cdot \int dk\, \exp\left[-\mathcal{D}t\left(k - \frac{ix}{2\mathcal{D}t}\right)^2\right] \cdot e^{\mathcal{D}t\left(\frac{ix}{2\mathcal{D}t}\right)^2}$$

$$= \frac{1}{2\pi}\, e^{-x^2/4\mathcal{D}t} \int_{-\infty}^{\infty} dk\, e^{-\mathcal{D}tk^2} = \frac{1}{2\pi} e^{-x^2/4\mathcal{D}t} \cdot \sqrt{\frac{\pi}{\mathcal{D}t}}$$

$$\hookrightarrow \boxed{W(x,t) = \frac{1}{\sqrt{4\pi\mathcal{D}t}}\, e^{-x^2/4\mathcal{D}t}} \qquad (1.1.28)$$

It is normalised

$$\int_{-\infty}^{\infty} W(x,t)\, dx = 1$$

- Transition probability

$$W_i(n) \equiv W(il, n\varepsilon) = \sum_j W_{ij}(n\varepsilon)\, W_j(0)$$

$$\Big\downarrow \text{ continuous limit}$$

$$\boxed{\underbrace{W(x_t,t)}_{\substack{\text{prob. distr.}\\ \text{at } t}} = \int_{-\infty}^{\infty} dx_0\, \underbrace{W(x_t,t|x_0,t_0)}_{\substack{\text{transition } t_0\to t\\ \text{probability}}}\, \underbrace{W(x_0,t_0)}_{\substack{\text{prob. distribution}\\ \text{at } t_0}}} \qquad (1.1.32)$$

Since $W(x,t)$ satisfies the diff. eq., so is $W(x_t t|x_0 t_0)$, and since

$$W(x_t,t) \xrightarrow[t\to t_0]{} W(x_0,t_0)$$

then

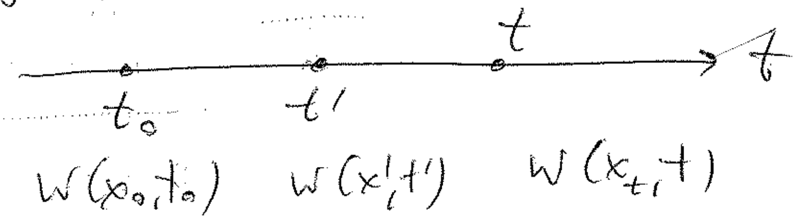
$$W(x_t,t\,|\,x_0,t_0) \underset{t\to t_0}{\Longrightarrow} \delta(x_t - x_0)$$

which gives the solution

$$\boxed{W(x_t,t\,|\,x_0 t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}}\exp\left[-\frac{(x_t-x_0)^2}{4D(t-t_0)}\right]} \quad (1.1.35)$$

It depends on $x_t - x_0$ and $t-t_0$ due to space and time homogeneity.

• Semi group property



$$w(x_t,t) = \int dx_0\, W(x_t,t\,|\,x_0 t_0)\, w(x_0,t_0)$$

$$\equiv \int dx'\, W(x_t,t\,|\,x' t')\, w(x',t')$$

$$\equiv \int dx'\,dx_0\, W(x_t,t\,|\,x' t')\, W(x' t'\,|\,x_0 t_0)\, w(x_0,t_0)$$

$$\hookrightarrow \boxed{\begin{gathered} W(x_t,t\,|\,x_0 t_0) = \int dx'\, W(x_t t\,|\,x' t')\, W(x' t'\,|\,x_0 t_0) \\ t_0 < t' < t \end{gathered}} \quad (1.1.45)$$

(Einstein – Smoluchowski – Kolmogorov – Chapman)(ESKC) relation

• Multidimensional Brownian motion

$$\cancel{w(x, n\varepsilon) = \sum_{i_1, i_2, \dots, i_k} [W(\varepsilon)]^n}$$

~~over all dimensions~~

It can go in one of the d directions (both $\pm\ell$); for one step over time ε the transition probability:

$$W(\vec{x}, \varepsilon) = \begin{cases} 1/2d, & |\bar{x}| \le \ell \\ 0, & \text{otherwise} \end{cases} \quad (= 1/2, 1D \mid = 1/4, 2D \mid = 1/6, 3D)$$

$\vec{x}$ — displacement

$$\vec{x} = \{n_1\ell, n_2\ell, \dots, n_d\ell\}$$

and
$$W(\vec{x}, \varepsilon) = \begin{cases} 1/d2, & \text{if } n_i \to n_i \pm 1 \text{ for any } i \\ 0, & \text{otherwise} \end{cases}$$

$$\equiv \frac{1}{2d} \sum_{k=1}^{d} \left[w(\bar{x} + \ell\bar{e}_k, \varepsilon) + w(\bar{x} - \ell\bar{e}_k, \varepsilon) \right],$$

where $\bar{e}_k$ are unit vectors in all d directions,

$$= \frac{1}{2d} \sum_{k=1}^{d} \left[\delta_{n_k, n_k+1} + \delta_{n_k, n_k-1} \right]$$

Here $W(\vec{x}, \varepsilon)$ represents a matrix of many dimensions:

$$W = \| W_{n_1 n_1'; n_2 n_2'; \dots; n_d n_d'} \|$$

Use discrete FT over $\vec{x}$ for the $w(\vec{x}, t)$ (~~which is periodic with the period of~~ ~~probability and is~~ ℓ

$$\cancel{W(\vec{x}, t) = \int_{-\pi/\ell}^{\pi/\ell} dp_1 dp_2 \dots dp_d \, \tilde{W}(\vec{p}, t) e^{i\vec{p}\vec{x}}}$$

• <u>Discrete FT</u> Consider 1Δ case. Large period N:

$$w(n)\ \big(\equiv w(n\ell)\big) \Rightarrow w(n+N')$$

$$\hookrightarrow\ w(n) = \frac{1}{N'}\sum_{j=1}^{N'} \tilde{w}_j\, e^{i2\pi jn/N'}$$

with $$\tilde{w}_j = \sum_{n=1}^{N'} w(n)\, e^{-i2\pi jn/N'}$$

Indeed,

$$\tilde{w}_j = \sum_{n=1}^{N'} e^{-i2\pi jn/N'}\ \frac{1}{N'}\sum_{j'=1}^{N'} \tilde{w}_{j'}\, e^{i2\pi j'n/N'}$$

$$= \sum_{j'} \tilde{w}_{j'} \underbrace{\left[\frac{1}{N'}\sum_{n=1}^{N'} e^{-i2\pi(j-j')n/N'}\right]}_{\delta_{jj'}} \equiv \tilde{w}_j\,,$$

and also

$$w(n) = \frac{1}{N'}\sum_{j=1}^{N'} e^{i2\pi jn/N'} \sum_{n'=1}^{N'} w(n')\, e^{-i2\pi jn'/N'}$$

$$= \sum_{n'} w(n') \underbrace{\left[\frac{1}{N'}\sum_{j} e^{i2\pi j(n-n')/N'}\right]}_{\delta_{nn'}} \equiv w(n)\,,$$

so it works.

Denote $\Delta p = \frac{2\pi}{N\ell}$, $x\ (=x_n) = n\ell$, then

$$\frac{2\pi jn}{N'} = \left(\frac{2\pi}{N'\ell}\cdot j\right)\left(n\ell\right) = p_j \cdot x_n = px\,,$$

$$p_j = \Delta p \cdot j$$

Replace $\tilde{w}_j$ with $= \cancel{\tilde{w}(p_j)\cdot\Delta p N'} = \tilde{w}(p_j)\,\frac{2\pi}{\ell}$. Then:

$$w(n) = \sum_{j=1}^{N'} \tilde{w}(p_j)\, \underbrace{\frac{2\pi}{N'\ell}}_{\Delta p}\, e^{ip_jx_n} = \sum_{j=1}^{N'} \tilde{w}(p_j)\,\Delta p\, e^{ip_jx_n}$$

$p_j \to p_1 = \frac{2\pi}{N'\ell}$ up to $p_{N'} = \frac{2\pi}{\ell}$, so that in $N' \to \infty$:

$$w(n) \to \int_0^{2\pi/\ell} \tilde{w}(p)\, e^{ipx_n}\, dp = \cancel{\int_{-\pi/\ell}^{\pi/\ell} \tilde{w}(p)\, e^{ipx}\, dp}$$

~~Since $\tilde{w}(p \pm \frac{2\pi}{\ell}) = \tilde{w}(p)$. Indeed. Ch~~, and

$$\tilde{w}(p) = \tilde{w}(p_j) \equiv \frac{\ell}{2\pi} \tilde{w}_j G = \frac{\ell}{2\pi} \sum_{n=1}^{N'} w(n)\, e^{-ip_j x_n},$$

i.e.

$$\tilde{w}(p) = \frac{\ell}{2\pi} \sum_{n=-\infty}^{\infty} w(x_n)\, e^{-ipx_n}$$

Here $\tilde{w}(p + \frac{2\pi}{\ell}) = \frac{\ell}{2\pi} \sum_n w(x_n)\, e^{i(p+\frac{2\pi}{\ell})x_n} = \tilde{w}(p)$

as $\frac{2\pi}{\ell} \cdot x_n = \frac{2\pi}{\ell} n\ell = 2\pi n$. This allows a change of variables (shift) in $w(n)$:

$$\boxed{w(x) = w(n\ell) \equiv \int_{-\pi/\ell}^{\pi/\ell} \tilde{w}(p)\, e^{ipx}\, dp}$$

$$\boxed{\tilde{w}(p) = \frac{\ell}{2\pi} \sum_n w(x_n) e^{-ipx_n}}$$

- Now we can write for the d-dimensional case:

$$\boxed{\begin{aligned} w(\vec{x}) &= \int_{-\pi/\ell}^{\pi/\ell} dp_1\, dp_2 \ldots dp_d\ \tilde{w}(\vec{p})\, e^{i\vec{p}\vec{x}} \\ \tilde{w}(\vec{p}) &= \left(\frac{\ell}{2\pi}\right)^d \sum_{n_1 n_2 \ldots n_d} w(\vec{x})\, e^{-i\vec{p}\vec{x}} \end{aligned}}$$

where $\vec{x} = \ell(n_1 \vec{e}_1 + \ldots + n_d \vec{e}_d)$, $\vec{p} = \frac{2\pi}{N\ell}(j_1 \vec{e}_1 + j_2 \vec{e}_2 + \ldots + j_d \vec{e}_d)$

~~With~~ so that

$$\vec{p}\cdot\vec{x} = \underbrace{\frac{2\pi}{N\ell}}_{\Delta p}(j_1 n_1 + \dots + j_d n_d)\cdot\ell = p_1 x_1 + p_2 x_2 + \dots + p_d x_d$$

- Define ~~translation~~ transition operator:

$$\hat{W}\, w(\vec{x}) = \frac{1}{2d}\sum_{k=1}^{d}\left[w(\vec{x}+\ell\vec{e}_k) + w(\vec{x}-\ell\vec{e}_k)\right]$$

$$\hat{W}\int (d^d p)\,\tilde{w}(\vec{p})\,e^{i\vec{p}\vec{x}} =$$

$$= \frac{1}{2d}\sum_{k=1}^{d}\int (d^d p)\,\tilde{w}(\vec{p})\left[e^{i\vec{p}(\vec{x}+\ell\vec{e}_k)} + e^{i\vec{p}(\vec{x}-\ell\vec{e}_k)}\right]$$

$$= \int (d^d p)\,\tilde{w}(\vec{p})\,e^{i\vec{p}\vec{x}}\left[\frac{1}{2d}\sum_{k=1}^{d}\left(e^{i(\vec{p}\cdot\vec{e}_k)\ell} + e^{-i(\vec{p}\cdot\vec{e}_k)\ell}\right)\right]$$

Here

$$\vec{p}\cdot\vec{e}_k = \frac{2\pi}{N\ell}\, j_k\,,$$

$$[\dots] = \frac{1}{2d}\sum_{k=1}^{d} 2\cos\Big(\underbrace{\frac{2\pi}{N\ell}\, j_k}_{p_k}\cdot\ell\Big) = \frac{1}{d}\sum_{k=1}^{d}\cos(p_k\ell)$$

This means, that

$$\hat{W}\, w(\vec{p}) = \lambda(\vec{p})\, w(\vec{p})$$

with

$$\lambda(\vec{p}) = \frac{1}{d}\sum_{k=1}^{d}\cos(p_k\ell)$$

- After N jumps we apply $\hat{W}$ N times $(t = N\varepsilon)$:

$$\hat{W}(\vec{x}, N\varepsilon) = \left[\hat{W}(\vec{x},\varepsilon)\right]^N$$

$$\hat{W}(\vec{x}, N\varepsilon)\, w(\vec{p}) = \left[\lambda(p)\right]^N w(\vec{p})$$

or ~~$W(\vec{x}, N\varepsilon)\, \omega(\vec{x})$~~ (since $\hat{W}$ acts only on e^{ipx}):

$$\hat{W}\, w(\vec{x}) = \int d\vec{p}\, \tilde{w}(p)\, e^{i\vec{p}\vec{x}}\, \lambda(\vec{p})$$

$$[\hat{W}]^2 w(\vec{x}) = \int d\vec{p}\, \tilde{w}(p)\, e^{i\vec{p}\vec{x}}\, \lambda^2(\vec{p})$$

$$\cdots$$

$$[W]^N w(\vec{x}) = \int d\vec{p}\, \tilde{w}(\vec{p})\, e^{i\vec{p}\vec{x}}\, \lambda^N(\vec{p}) \equiv W(\vec{x}, N\varepsilon)$$

Calculate

$$[\lambda(\vec{p})]^N = \exp[N \ln \lambda(\vec{p})] = \exp\Big[\underbrace{N}_{t/\varepsilon} \ln\Big(\frac{1}{d} \sum_{k=1}^{d} \cos(p_k \ell)\Big)\Big]$$

We tend $\ell \to 0$, $N \to \infty$, then

$$\cos(p_k \ell) = 1 - \frac{1}{2}(p_k \ell)^2 + O(\ell^4)$$

$$\frac{1}{d} \sum_{k=1}^{d} \cos(p_k \ell) = 1 - \frac{\ell^2}{2d} p^2 + O(\ell^4)$$

$$\hookrightarrow [\lambda(p)]^N = \exp\Big[\frac{t}{\varepsilon} \ln\Big(1 - \frac{\ell^2}{2d} p^2 + O(\ell^4)\Big)\Big]$$

$$\simeq \exp\Big[\frac{t}{\varepsilon}\Big(-\frac{\ell^2}{2d} p^2\Big)\Big] = \exp\Big[-t \underbrace{\Big(\frac{\ell^2}{2\varepsilon d}\Big)}_{\mathcal{D}} p^2\Big] = e^{-\mathcal{D} t p^2}$$

where
$$\boxed{\mathcal{D} = \frac{\ell^2}{2\varepsilon d} \quad (\text{when } \varepsilon \to 0,\ \ell \to 0)}$$

- Therefore,

$$w(\vec{x}_N, t) = \int d\vec{p}\, \tilde{w}(\vec{p})\, e^{i\vec{p}\vec{x}}\, e^{-\mathcal{D} t p^2}$$

Here $\tilde{w}(p)$ represents the $t=0$ distribution as we acted on it with $\hat{w}$. Initially, $w(\vec{x}) = \delta_{n_1 0}\delta_{n_2 0}\ldots\delta_{n_p 0}$, and

$$\tilde{w}(\vec{p}) = \left(\frac{\ell}{2\pi}\right)^d \sum_{n_1\ldots n_d} e^{-i\vec{p}\vec{x}_n}\,\delta_{n_1 0}\ldots\delta_{n_p 0} \equiv \left(\frac{\ell}{2\pi}\right)^d,$$

so that

$$w(\vec{x}_n, t) = \left(\frac{\ell}{2\pi}\right)^d \int d\vec{p}\, e^{i\vec{p}\vec{x}}\, e^{-\mathcal{D}t\vec{p}^{\,2}}$$

- Calculating the multidimensional $\vec{p}$-integral.

$$\left(\frac{1}{2\pi}\right)^d \int d\vec{p}\, e^{i\vec{p}\vec{x}} e^{-\mathcal{D}t\vec{p}^{\,2}} = \prod_{k=1}^{d} \frac{1}{2\pi}\int dp_k\, e^{ip_k x_k} e^{-\mathcal{D}t p_k^2}$$

$$= \prod_k \frac{1}{\sqrt{4\pi\mathcal{D}t}}\, e^{-x_k^2/4\mathcal{D}t} = \left(\frac{1}{4\pi\mathcal{D}t}\right)^{d/2} e^{-x^2/4\mathcal{D}t}$$

[Here the p_k integration was extended to $\pm\infty$ due to $e^{-\mathcal{D}tp_k^2}$.]

- Normalisation of $w(\vec{x}, t)$ should be changed as compared of that of $w(\vec{x}_n, t)$:

$$\sum_{n_1 n_2 \ldots n_d} w(x_n, t) = 1 \to \sum_{n_1\ldots n_d} w(x_n, t)\,\ell^d =$$

$$= \int d\vec{x}\, w(\vec{x}, t) = \ell^d$$

Since it $w(\vec{x}, t)$ should be normalised to 1, we should accept:

$$\boxed{w(x_n, t) \to \frac{1}{\ell^d}\, w(x_n, t)}$$

and hence

$$\boxed{w(\vec{x}, t) = \frac{1}{(4\pi\mathcal{D}t)^{d/2}}\, e^{-x^2/4\mathcal{D}t}}$$

• 1D problem with different left and right probabilities

$$\hat{W}\, w(x) = p\, w(x+l) + q\, w(x-l),$$

$$p + q = 1$$

If $$w(x) = \int_{-\pi/l}^{\pi/l} \tilde{w}(g)\, e^{igx}\, dg\,,$$

$$\tilde{w}(g) = \frac{l}{2\pi} \sum_n w(x_n)\, e^{-igx_n}\,, \quad x_n = nl\,,$$

then

$$\hat{W}\, w(x) = \int_{-\pi/l}^{\pi/l} dg\, \tilde{w}(g) \left\{ p e^{igl} + q e^{-igl} \right\} e^{igx}$$

$$\{\ldots\} = p \cancel{\left[e^{ipl} - e^{-ipl}\right] + e^{-ipl}} = p(c+is) + q(c-is)$$

$$= \underset{\substack{\| \\ 1}}{(p+q)} \cos gl + i(p-q)\sin gl = \cos gl + i(p-q)\sin gl$$

$$\hookrightarrow \hat{W}\, w(x) = \int_{-\pi/l}^{\pi/l} dg\, \tilde{w}(g)\, \lambda(g)\, e^{igx}\,, \quad \lambda(g) = \cos gl + i(p-q)\sin gl$$

$$W^N \underbrace{w(x)}_{\text{initial}} = \int dg\, [\lambda(g)]^N\, \tilde{w}(g)\, e^{igx}\,,$$

where

$$\cancel{[\lambda(g)]^N = \left[1 - \frac{1}{2} g^2 l^2 + O(l^4)\right] + i(p-q)\left[gl + O(l^3)\right]}$$

$$\cancel{= 1 - \frac{1}{2} g^2 l^2 + i(p-q)\, gl + O(l^3) =}$$

$$\cancel{= \exp\left\{ \ln\left[1 - \frac{l^2}{2} g^2 + i(p-q)\, gl + O(l^3)\right]\right\}}$$

$$\simeq \cancel{\exp\left\{+i(p-q)gl - \frac{l^2}{2}g^2\right\}}$$

$$\left(\lambda(g)\right)^N = \exp\left\{N \ln\left[\cos gl + i(p-q)\sin gl\right]\right\}$$

$$\simeq \exp\left\{N \ln\left[1 - \frac{g^2 l^2}{2} + i(p-q)gl + O(l^3)\right]\right\}$$

$$\simeq \exp\left\{N\left[-\frac{g^2 l^2}{2} + i(p-q)gl\right]\right\} = \exp\left[\frac{t}{\varepsilon}\left[-\frac{g^2 l^2}{2} + i(p-q)gl\right]\right]$$

$$\to \exp\left[-t\left(g^2 \underbrace{\frac{l^2}{2\varepsilon}}_{D} - i\underbrace{\frac{(p-q)l}{\varepsilon}}_{v} g\right)\right] = e^{-t(Dg^2 - ivg)}$$

Therefore ($x_n = nl$ here):

$$w(x, N\varepsilon) = \hat{W}^N \underbrace{w(x)}_{\text{initial}} = \int_{-\pi/l}^{\pi/l} dg\, \tilde{w}(g) e^{igx} e^{-t(Dg^2 - ivg)}$$

$$= \int_{-\pi/l}^{\pi/l} dg\, \tilde{w}(g)\, e^{ig(x+vt)}\, e^{-tg^2 D}$$

Initially the particle was at 0, i.e.

$$w(x) = \delta_{n0} \to \tilde{w}(g) = \frac{l}{2\pi}\sum_n \delta_{n0} e^{-igx_n} = \frac{l}{2\pi}$$

$$\hookrightarrow w(x, N\varepsilon) = \frac{l}{2\pi}\int_{-\pi/l}^{\pi/l} dg\, e^{ig(x+vt)}\, e^{-tDg^2}$$

$$= \cancel{\frac{l}{2}}\, l \cdot \frac{1}{\sqrt{4\pi D t}}\, e^{-(x+vt)^2/4Dt}$$ for $x = x_n$

Continuous limit: $\boxed{w(x,t) = \frac{1}{l} w(x_n, N\varepsilon) \equiv \frac{1}{\sqrt{4\pi D t}}\, e^{-\frac{(x+vt)^2}{4Dt}}}$

It satisfies the following DE: $(x' = x + vt)$:

$$\frac{\partial w}{\partial t} = \underbrace{\frac{\partial}{\partial t}\begin{bmatrix}\text{old} \\ \text{result}\end{bmatrix}}_{\frac{\partial w(x')}{\partial t} \equiv D \frac{\partial^2 w(x')}{\partial x'^2}} + \frac{\partial w}{\partial x'} \underbrace{\frac{\partial x'}{\partial t}}_{v} = v \frac{\partial w}{\partial x} + D \frac{\partial^2 w}{\partial x^2}$$

since $\partial / \partial x' = \partial / \partial x$.