

(1.2) Wiener path integrals & stochastic processes -45-
The Fokker-Planck eq.

$W(x_t, t | x_\tau, \tau)$ - transition probability $\tau \rightarrow t$

Assumptions:

$$\lim_{t \rightarrow \tau} \left\langle \frac{x_t - x_\tau}{t - \tau} \right\rangle = A(x_\tau, \tau) \quad (\text{"mean velocity"}) \quad (1.2.15)$$

$$\lim_{t \rightarrow \tau} \left\langle \frac{(x_t - x_\tau)^2}{t - \tau} \right\rangle = 2B(x_\tau, \tau) \quad (1.2.16)$$

$$\lim_{t \rightarrow \tau} \left\langle \frac{(x_t - x_\tau)^3}{t - \tau} \right\rangle = 0 \quad (1.2.17)$$

$$\langle f(x_t - x_\tau) \rangle = \int dx_t f(x_t - x_\tau) W(x_t, t | x_\tau, \tau)$$

We would like to derive an eq. for W . It satisfies the ESKC:

$$W(x_t, t | x_0, 0) = \int dx_\tau W(x_\tau, \tau | x_0, 0) W(x_t, t | x_\tau, \tau)$$

Multiply it by an arbitrary $g(x)$ which satisfies:

$$g(x) \xrightarrow{x \rightarrow \pm\infty} 0, \quad g'(x) \xrightarrow{x \rightarrow \pm\infty} 0 \quad (1.2.18)$$

$$\begin{aligned} \int_{-\infty}^{\infty} g(x_t) W(x_t, t | x_0, 0) dx_t &= \\ &= \int dx_\tau \int dx_t g(x_t) W(x_t, t | x_\tau, \tau) W(x_\tau, \tau | x_0, 0) \end{aligned} \quad (1.2.19)$$

Expand $g(x)$:

$$\begin{aligned} g(x_t) - g(x_\tau) &= (x_t - x_\tau) g'(x_\tau) + \frac{1}{2} (x_t - x_\tau)^2 g''(x_\tau) + \\ &+ \frac{1}{6} (x_t - x_\tau)^3 g'''(\xi), \end{aligned}$$

where $\xi \in [x_\tau, x_t]$. Substitute this in (1.2.19):

$$\text{LHS} = g(x_\tau) \int_{-\infty}^{\infty} W dx_t + \int_{-\infty}^{\infty} g(x_t) W(x_t, t | x_0, 0) dx_t$$

$$RHS = \int dx_\tau dx_t \underbrace{g(x_\tau) W(x_t, t | x_\tau, \tau) W(x_\tau, \tau | x_0, 0)}$$

$$= \int dx_\tau \left[\underbrace{\int dx_t W(x_t, t | x_\tau, \tau)}_1 \right] g(x_\tau) W(x_\tau, \tau | x_0, 0)$$

$$+ \int dx_\tau dx_t (x_t - x_\tau) W(x_\tau, \tau | x_0, 0) W(x_t, t | x_\tau, \tau) g'(x_\tau)$$

$$\int dx_\tau \langle x_t - x_\tau \rangle W(x_\tau, \tau | x_0, 0)$$

$$+ \frac{1}{2} \int dx_\tau dx_t (x_t - x_\tau)^2 W(x_\tau, \tau | x_0, 0) W(x_t, t | x_\tau, \tau) g''(x_\tau)$$

$$\frac{1}{2} \int dx_\tau \langle (x_t - x_\tau)^2 \rangle W(x_\tau, \tau | x_0, 0)$$

$$+ \frac{1}{6} \int dx_\tau dx_t (x_t - x_\tau)^3 W(x_t, t | x_\tau, \tau) W(x_\tau, \tau | x_0, 0) g'''(x_\tau)$$

$$\frac{1}{6} \int dx_\tau \langle (x_t - x_\tau)^3 \rangle W(x_\tau, \tau | x_0, 0)$$

$$= \int dx_\tau g(x_\tau) W(x_\tau, \tau | x_0, 0) + \int dx_\tau g'(x_\tau) \langle x_t - x_\tau \rangle W(x_\tau, \tau | x_0, 0)$$

$$+ \frac{1}{2} \int dx_\tau g''(x_\tau) \langle (x_t - x_\tau)^2 \rangle W(x_\tau, \tau | x_0, 0)$$

$$+ \frac{1}{6} \int dx_\tau g'''(x_\tau) \langle (x_t - x_\tau)^3 \rangle W(x_\tau, \tau | x_0, 0)$$

Take the 1st term in the LHS and divide by $t - \tau$:

$$\frac{\int dx_t g(x_t) W(x_t, t | x_0, 0) - W(x_0, t | x_0, 0)}{t - \tau} \rightarrow \frac{\partial W(x_0, t)}{\partial t}$$

-47-

$$LHS = \frac{\left[\int dx_t g(x_t) W(x_t | x_0, 0) - \int dx_\tau g(x_\tau) W(x_\tau | x_0, 0) \right]_{t \rightarrow \tau}}{t - \tau}$$

$$= \int dx g(x) \frac{W(x_t | x_0, 0) - W(x_\tau | x_0, 0)}{t - \tau} + \int dx_t g(x_t) \frac{\partial W(x_t | x_0, 0)}{\partial t}$$

$$RHS = \int dx_\tau g'(x_\tau) \underbrace{\left[\frac{\langle x_t - x_\tau \rangle}{t - \tau} \right]}_{\rightarrow A(x_\tau, \tau)} W(x_\tau, \tau | x_0, 0)$$

$$+ \frac{1}{2} \int dx_\tau g''(x_\tau) \underbrace{\left[\frac{\langle (x_t - x_\tau)^2 \rangle}{t - \tau} \right]}_{\rightarrow 2B(x_\tau, \tau)} W(x_\tau, \tau | x_0, 0) + \left(\begin{matrix} \text{3rd term} \\ \rightarrow 0 \end{matrix} \right)$$

$$\xrightarrow{t} \int dx_t g'(x_t) A(x_t, t) W(x_t, t | x_0, 0)$$

$$+ \int dx_t g''(x_t) B(x_t, t) W(x_t, t | x_0, 0) = \text{By parts}$$

$$= \left\{ \underbrace{g(x_t)}_0 \frac{\partial}{\partial x_t} [A(x_t, t) W(x_t, t | x_0, 0)] \right\}_{-\infty}^{\infty} - \int dx_t g(x_t) \frac{\partial}{\partial x_t} [A(x_t, t) W(x_t, t | x_0, 0)]$$

$$+ \left\{ \underbrace{g'(x_t)}_0 \frac{\partial}{\partial x_t} [B(x_t, t) W(x_t, t | x_0, 0)] \right\}_{-\infty}^{\infty} - \int g'(x_t) \frac{\partial}{\partial x_t} [B(x_t, t) W(x_t, t | x_0, 0)] dx_t \Bigg\} = \left(\begin{matrix} \text{once} \\ \text{again for} \\ \text{the 2nd term} \end{matrix} \right)$$

$$= - \int dx_t g(x_t) \frac{\partial}{\partial x_t} [A(x_t, t) W(x_t, t | x_0, 0)] + \left\{ \underbrace{g(x_t)}_0 \frac{\partial^2}{\partial x_t^2} [B(x_t, t) W(x_t, t | x_0, 0)] \right\}_{-\infty}^{\infty}$$

$$- \int g(x_t) \frac{\partial^2}{\partial x_t^2} [B(x_t, t) W(x_t, t | x_0, 0)] dx_t \Bigg\} =$$

$$= - \int dx_t g(x_t) \left[\frac{\partial}{\partial x_t} [AW] - \frac{\partial^2}{\partial x_t^2} [BW] \right]$$

Since LHS = RHS for any $g(x)$, we obtain:

$$\boxed{\frac{\partial W}{\partial t} + \frac{\partial}{\partial x_t} (AW) - \frac{\partial^2}{\partial x_t^2} (BW) = 0} \quad (1.2.21)$$

which is the Fokker-Planck (2nd Kolmogorov) equation.

If $A=0$, $B=D=\text{Constant}$, we obtain

$$\frac{\partial W}{\partial t} = D \frac{\partial^2 W}{\partial x_t^2} \quad \text{diffusion eq.}$$

1.2.2. Brownian particle under external force

$$m \ddot{x} + \gamma \dot{x} = F + \phi$$

Over long times $t \gg m/\gamma$ the $m \ddot{x}$ term can be dropped.

$$\text{LD } \ddot{x} = F + \phi$$

(1.2.25)

Here we consider the harmonic force:

$$\dot{x}(t) + kx(t) = \phi(t)$$

(1.2.31)

(Ornstein-Uhlenbeck process)

$$\text{Compare this with } \dot{y} = \phi(t) \rightarrow \dot{y} = \dot{x} + kx$$

$$\boxed{y(t) = x(t) + k \int_0^t d\tau x(\tau)} \quad , \quad \boxed{y(0) = x(0)} \quad (1.2.34)$$

$$\text{Reverseley, } \dot{x} + kx = 0 \rightarrow x = C e^{-kt}$$

$$\dot{x} + kx = \dot{y}(t) \rightarrow x(t) = C(t) e^{-kt}$$

$$\dot{C} e^{-kt} - k C e^{-kt} + k C e^{-kt} = \dot{y}$$

$$\dot{C} = \dot{y} e^{kt} \rightarrow C(t) = \int_0^t d\tau \dot{y}(\tau) e^{k\tau} + C'$$

$$= y(t) e^{kt} - (k) \int_0^t d\tau y(\tau) e^{k\tau} = y(t) e^{kt} + k \int_0^t y(\tau) e^{k\tau} d\tau$$

so that $x(0) = c(0) - y(0) = y(0)$

$$= c' + y(\tau) e^{k\tau} \Big|_0^t - \int_0^t d\tau y(\tau) k e^{k\tau} =$$

$$= c' + y(t) e^{kt} - y(0) - k \int_0^t y(\tau) e^{k\tau} d\tau$$

$$\hookrightarrow x(t) = c' e^{-kt} + y(t) - y(0) e^{-kt} - k \int_0^t y(\tau) e^{k(\tau-t)} d\tau$$

c' is obtained from $x(0) = y(0)$:

$$x(0) = c' + y(0) - y(0) = c' \rightarrow$$

$$\boxed{x(t) = y(t) - k \int_0^t e^{-k(t-\tau)} y(\tau) d\tau} \quad (1.2.35)$$

• Integration is to be understood in terms of the stochastic calculus. For linear functions integration by parts is legitimate.

• If we know probability density for the process $y(t)$,

$$d_w y(t) = \exp \left[- \int_0^t d\tau \dot{y}(\tau)^2 \right] \prod_{\tau=0}^t \frac{dy(\tau)}{\sqrt{\pi} d\tau} \quad (4D=1)$$

Then probability density for $x(t)$ related to $y(t)$ via (1.2.35) is simply given by the change of coordinates:

$$d_w y(t) = \mathcal{J} \exp \left[- \int_0^t d\tau (\dot{x} + kx)^2 \right] \prod \frac{dx(\tau)}{\sqrt{\pi} d\tau}$$

the Jacobian $|\partial y / \partial x|$

The Jacobian was calculated earlier for a general change of variables

$$\left[\begin{aligned} y(t) &= x(t) + \lambda \int_0^t ds k(s) x(s) & (1.1.122) \\ \mathcal{J} &= \exp \left[\frac{\lambda}{2} \int_0^t ds k(s) \right] & (1.1.127) \end{aligned} \right]$$

So in our case

$$y = \exp \left[-\frac{k}{2} \int_0^t ds \cdot 1 \right] = e^{kt/2}$$

The initial points of $x(t)$, $y(t)$ are fixed to $x(0) = y(0)$; we put $x_t = y_t$ for the final points as well.

$$\hookrightarrow W(x_t, t | x_0, 0) = e^{kt/2} \int_{C[x_0, 0; x_t, t]} \prod_{\tau=0}^t \frac{dx(\tau)}{\sqrt{\pi} d\tau} \exp \left[- \int_0^t d\tau (\ddot{x} + kx)^2 \right]$$

Here

$$\begin{aligned} \int_0^t (\ddot{x} + kx)^2 d\tau &= \int_0^t (\ddot{x}^2 + 2kx\ddot{x} + k^2x^2) d\tau = \int_0^t \ddot{x}^2 d\tau + \underbrace{2k \int_0^t d\tau \cdot x \cdot \frac{dx}{d\tau}}_{k \int_0^t d(x^2)} \\ &+ k^2 \int_0^t x^2 d\tau = k(x_t^2 - x_0^2) + \int_0^t \ddot{x}^2 d\tau + k \int_0^t x^2 d\tau \end{aligned}$$

and we obtain:

$$\begin{aligned} W(x_t, t | x_0, 0) &= e^{kt/2 - k(x_t^2 - x_0^2)} \int_{C[x_0, 0; x_t, t]} \prod_{\tau=0}^t \frac{dx(\tau)}{\sqrt{\pi} d\tau} \exp \left[- \int_0^t \ddot{x}^2 d\tau - \int_0^t d\tau kx^2 \right] \\ &= \int_{C[x_0, 0; x_t, t]} d_w x(\tau) \exp \left[- \int_0^t d\tau k^2 x(\tau)^2 \right] \quad (1.2.38) \end{aligned}$$

[this is the integral from Example 1.5 for $p(t) \equiv k^2$]

• General non-stationary and non-linear external force

$$\ddot{x}(t) + f(x(t), t) = \phi(t) \quad (1.2.39)$$

$$\hookrightarrow \ddot{y} = \ddot{x} + f \rightarrow y(t) = x(t) + \int_0^t f(x(\tau), \tau) d\tau \quad (1.2.40)$$

The Jacobian in this case after discretisation:

~~$$y_1 = x_1 + \frac{1}{2} \varepsilon$$~~

$$y_i = x_i + \left[f(x_1, \varepsilon) + f(x_2, 2\varepsilon) + \dots + \frac{1}{2} f(x_N, N\varepsilon) \right] \varepsilon$$

$$y_1 = x_1 + \frac{1}{2} f(x_1, \varepsilon) \varepsilon$$

$$y_2 = x_2 + \left[f(x_1, \varepsilon) + \frac{1}{2} f(x_2, 2\varepsilon) \right] \varepsilon$$

$$\boxed{\varepsilon = \tau/N}$$

$$\left| \frac{\partial y}{\partial x} \right| = \begin{pmatrix} 1 + \frac{\varepsilon}{2} f'(x_1, \varepsilon) & 0 & 0 & \dots \\ f'(x_1, \varepsilon) \varepsilon & 1 + \frac{\varepsilon}{2} f'(x_2, 2\varepsilon) & 0 & \dots \\ f'(x_1, \varepsilon) \varepsilon & f'(x_2, 2\varepsilon) \varepsilon & 1 + \frac{\varepsilon}{2} f'(x_3, 3\varepsilon) & 0, \dots \\ \vdots & \vdots & \vdots & \ddots \\ f'(x_1, \varepsilon) \varepsilon & f'(x_2, 2\varepsilon) \varepsilon & \dots & 1 + \frac{\varepsilon}{2} f'(x_N, N\varepsilon) \end{pmatrix}$$

$$= \prod_{i=1}^N \left[1 + \frac{\varepsilon}{2} f'(x_i, \varepsilon) \right] \Rightarrow \prod_{i=1}^N \exp \left[\frac{\varepsilon}{2} f'(x_i, \varepsilon) + O(\varepsilon^2) \right]$$

$$\hookrightarrow \exp \left[\frac{1}{2} \sum_{i=1}^N \varepsilon f'(x_i, \varepsilon) \right] \rightarrow \exp \left[\frac{1}{2} \int_0^t f'(x_t, \tau) d\tau \right] \quad (1.2.42)$$

where $f' = \frac{\partial f}{\partial x}$.

Therefore,

$$W(x_t, t | x_0, 0) = \int_{C[x_0, 0; x_t, t]} \prod_{\tau=0}^t \frac{dx(\tau)}{\sqrt{u} d\tau} \exp \left[- \underbrace{\int_0^t d\tau \dot{y}(\tau)^2}_{\int_0^t d\tau [\dot{x} + f(x(\tau), \tau)]^2} \right] \cdot J \quad (1.2.43)$$

• Brownian particles with interactions

Two particles, no interaction:

$$\ddot{y}_1 = \phi_1; \quad \ddot{y}_2 = \phi_2$$

(1.2.44)

$$W(y_{1t}, y_{2t} | y_{10}, y_{20}) = \int_{C[y_{10}, y_{1t}]} d_W y(\tau) \int_{C[y_{20}, y_{2t}]} d_W y(\tau)$$

$$= W(y_{1t}^t | y_{10}^0) W(y_{2t}^t | y_{20}^0) \quad (1.2.45)$$

a product (since they are entirely independent).

Let now 2 particles (x-particles) do interact:

$$\begin{cases} \dot{x}_1 + k_{11}x_1 + k_{12}x_2 = \phi_1 \\ \dot{x}_2 + k_{21}x_1 + k_{22}x_2 = \phi_2 \end{cases} \quad (1.2.46)$$

and $\dot{X} + kX = \Phi$, $k = \begin{pmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{pmatrix}$, $X = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$, $\Phi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$
 $\dot{y} = \Phi$, $y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$

$$\hookrightarrow \dot{y} = \dot{X} + kX \rightarrow y(t) = x(t) + k \int_0^t x(s) ds \quad (1.2.52)$$

all via vectors and matrices.

The Jacobian: - the same as above but now with 2×2 matrices:

$$y_i = x_i + k\varepsilon [x_1 + x_2 + \dots + \frac{1}{2}x_N]$$

$$J = \left| \frac{\partial y_i}{\partial x_j} \right| = \begin{vmatrix} 1 + \frac{1}{2}k\varepsilon & 0 & \dots & 0 \\ k\varepsilon & 1 + \frac{1}{2}k\varepsilon & 0 & \dots \\ k\varepsilon & k\varepsilon & 1 + \frac{1}{2}k\varepsilon & 0 \\ \vdots & \vdots & \vdots & \ddots \end{vmatrix} = \prod_{i=1}^N \left(1 + \frac{1}{2}k\varepsilon \right)$$

$$= \prod_{i=1}^N \exp\left(\frac{1}{2}k\varepsilon\right) = \prod_{i=1}^N \begin{vmatrix} 1 + \frac{1}{2}k_{11}\varepsilon & \frac{1}{2}k_{12}\varepsilon \\ \frac{1}{2}k_{21}\varepsilon & 1 + \frac{1}{2}k_{22}\varepsilon \end{vmatrix}$$

$$= \prod_{i=1}^N \left\{ \left(1 + \frac{1}{2}k_{11}\varepsilon\right) \left(1 + \frac{1}{2}k_{22}\varepsilon\right) - \frac{1}{4}k_{12}k_{21}\varepsilon^2 \right\} \rightarrow \exp \left[\frac{1}{2}\varepsilon \sum_{i=1}^N (k_{11} + k_{22}) \right]$$

$$1 + \frac{1}{2}(k_{11} + k_{22})\varepsilon + O(\varepsilon^2)$$

$$= \exp \left[\frac{1}{2}\varepsilon N \cdot \text{Tr} k \right] = e^{t \text{Tr} k / 2}$$

$$(1.2.54)$$

Therefore,

$$W(\vec{x}_t | \vec{x}_0, t) = e^{\frac{t}{2} \text{Tr}(k)} \int_{C[\vec{x}_0, \vec{x}_t]} \prod \frac{dx_1(\tau)}{\sqrt{\pi} d\tau} \prod \frac{dx_2(\tau)}{\sqrt{\pi} d\tau} \times \exp \left[- \int_0^t \underbrace{(\dot{x}(s) + k x(s))^2 ds} \right] \quad (1.2.55)$$

$$\sum_{i=1}^2 \left[\dot{x}_i(s) + \sum_{j=1}^2 k_{ij} x_j(s) \right]^2$$

• Interacting k particles subject to general forces

$$\ddot{x}_i(t) + f_i(x(t), t) = \Phi_i(t) \quad , \quad i = 1, \dots, k$$

In vector/matrix form:

$$\ddot{x}(t) + f(x(t), t) = \Phi(t) \equiv \ddot{y}(t) \Rightarrow \{y_i^j, x_i^j\} \quad (j = \text{time})$$

~~$$y = \begin{pmatrix} \partial y \\ \partial x \end{pmatrix} = \begin{pmatrix} \partial y^1 / \partial x^1 & \partial y^1 / \partial x^2 & \dots & \partial y^1 / \partial x^k \\ \partial y^2 / \partial x^1 & \partial y^2 / \partial x^2 & \dots & \partial y^2 / \partial x^k \\ \vdots & \vdots & \ddots & \vdots \\ \partial y^k / \partial x^1 & \partial y^k / \partial x^2 & \dots & \partial y^k / \partial x^k \end{pmatrix} \quad \vec{y}(t) = \vec{x}(t) + \int_0^t \vec{f}(\vec{x}, s) ds$$~~

$$y_i^j = x_i^j + \left[f_i(\vec{x}^1, \varepsilon) + f_i(\vec{x}^2, 2\varepsilon) + \dots + \frac{1}{2} f_i(\vec{x}^N, N\varepsilon) \right] \varepsilon$$

$$J = \begin{vmatrix} (\partial y^1 / \partial x^1) & 0 & \dots & \dots \\ (\partial y^2 / \partial x^1) & (\partial y^2 / \partial x^2) & 0 & \dots \\ \vdots & \vdots & \ddots & \vdots \\ (\partial y^{(N)} / \partial x^1) & (\partial y^{(N)} / \partial x^2) & \dots & (\partial y^{(N)} / \partial x^{(N)}) \end{vmatrix}$$

where $\left(\frac{\partial y^{(j)}}{\partial x^{(i)}} \right) = \begin{vmatrix} \partial y_1^{(j)} / \partial x_1^{(i)} & \partial y_1^{(j)} / \partial x_2^{(i)} & \dots & \partial y_1^{(j)} / \partial x_k^{(i)} \\ \partial y_2^{(j)} / \partial x_1^{(i)} & \dots & \dots & \dots \\ \vdots & \vdots & \ddots & \vdots \\ \partial y_k^{(j)} / \partial x_1^{(i)} & \dots & \dots & \partial y_k^{(j)} / \partial x_k^{(i)} \end{vmatrix}$

-54-

$$= \begin{pmatrix} 1 + \frac{1}{2} \frac{\partial f_1}{\partial x_1} \varepsilon & \frac{1}{2} \frac{\partial f_1}{\partial x_2} \varepsilon & \frac{1}{2} \frac{\partial f_1}{\partial x_3} \varepsilon & \dots & \frac{1}{2} \frac{\partial f_1}{\partial x_k} \varepsilon \\ \frac{1}{2} \frac{\partial f_i}{\partial x_1} \varepsilon & 1 + \frac{1}{2} \frac{\partial f_i}{\partial x_2} \varepsilon & \dots & \dots & \frac{1}{2} \frac{\partial f_i}{\partial x_k} \varepsilon \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \frac{1}{2} \frac{\partial f_i}{\partial x_1} \varepsilon & \frac{1}{2} \frac{\partial f_i}{\partial x_2} \varepsilon & \dots & \dots & 1 + \frac{1}{2} \frac{\partial f_i}{\partial x_k} \varepsilon \end{pmatrix}$$

We differentiate only w.r.t to the j -th time: (diagonal matrices);

~~$y_i^1 = x_i^1 + \frac{1}{2} f_i(x_i^1, \varepsilon) \varepsilon$~~

$$y_i^1 = x_i^1 + \frac{1}{2} f_i(x_i^1, \varepsilon) \varepsilon$$

$$y_i^2 = x_i^2 + \left[f_i(x_i^1, \varepsilon) + \frac{1}{2} f_i(x_i^2, 2\varepsilon) \right] \varepsilon$$

$$y_i^3 = x_i^3 + \left[f_i(x_i^2, \varepsilon) + \frac{1}{2} f_i(x_i^2, 2\varepsilon) + \frac{1}{2} f_i(x_i^3, 3\varepsilon) \right] \varepsilon$$

So, the $j=1$ block is ($f_i^j \leftarrow j = \text{time}$)

$$A^1(\varepsilon) = \begin{pmatrix} 1 + \frac{1}{2} \frac{\partial f_1^1}{\partial x_1} \varepsilon & \frac{1}{2} \frac{\partial f_1^1}{\partial x_2} \varepsilon & \frac{1}{2} \frac{\partial f_1^1}{\partial x_3} \varepsilon & \dots & \frac{1}{2} \frac{\partial f_1^1}{\partial x_k} \varepsilon \\ \frac{1}{2} \frac{\partial f_2^1}{\partial x_1} \varepsilon & 1 + \frac{1}{2} \frac{\partial f_2^1}{\partial x_2} \varepsilon & \frac{1}{2} \frac{\partial f_2^1}{\partial x_3} \varepsilon & \dots & \frac{1}{2} \frac{\partial f_2^1}{\partial x_k} \varepsilon \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & 1 + \frac{1}{2} \frac{\partial f_k^1}{\partial x_k} \varepsilon \end{pmatrix}$$

$$\approx \left(\text{up to the linear in } \varepsilon \text{ terms} \right) \approx 1 + \frac{1}{2} \sum_{i=1}^k \frac{\partial f_i^1}{\partial x_i} \varepsilon$$

At time $j=2$ (the 2nd diagonal element in the matrix J we would have

$$A^2(\varepsilon) = 1 + \frac{1}{2} \sum_{i=1}^k \frac{\partial f_i^2}{\partial x_i} \varepsilon, \text{ etc.}$$

So

$$J = \prod_{j=1}^N A^j(\varepsilon) = \prod_{j=1}^N \left(1 + \frac{1}{2} \sum_{i=1}^k \frac{\partial f_i^j}{\partial x_i} \varepsilon \right) \approx$$

-35-

$$\approx \prod_{j=1}^N \exp \left[\frac{1}{2} \sum_{i=1}^k \frac{\partial f_i^j}{\partial x_i} \varepsilon \right] = \exp \left[\frac{1}{2} \sum_{i=1}^k \left(\sum_{j=1}^N \frac{\partial f_i^j}{\partial x_i} \varepsilon \right) \right]$$

$$\hookrightarrow \exp \left[\frac{1}{2} \sum_{i=1}^k \int_0^t \frac{\partial f_i(\vec{x}(s), s)}{\partial x_i} ds \right]$$

and then

$$W(\vec{x}_t, t | \vec{x}_0, 0) = \int_{C[\vec{x}_0, 0; \vec{x}_t, t]} \prod \frac{dx_i(\tau)}{\sqrt{\pi} d\tau} \dots \prod \frac{dx_k(\tau)}{\sqrt{\pi} d\tau}$$

$$\times \exp \left[\frac{1}{2} \sum_{i=1}^k \int_0^t \frac{\partial f_i}{\partial x_i} ds \right] \exp \left[- \sum_{i=1}^k \int_0^t ds \left(\dot{x}_i(s) + \sum_{j=1}^N f_i^j(x(s), s) \right)^2 \right]$$

(1.2.58)

1.2.4. Brownian particles with inertia

• 2nd order DE

$$m \ddot{x} + \gamma \dot{x} = F + \phi$$

is first changed into two 1st order eqs:

$$\begin{cases} \dot{x} - v = 0 \\ \dot{v} + \frac{\gamma}{m} v - \frac{F}{m} = \frac{1}{m} \phi \end{cases} \quad (1.2.59)$$

• We introduce "temperatures"

$$\begin{cases} \dot{v} + \frac{\gamma}{m} v - \frac{1}{m} f = T_1 \frac{1}{m} \phi_1 \\ \dot{x} - v = T_2 \phi_2 \end{cases} \quad (1.2.60)$$

[$T_2 \rightarrow 0$ and $T_1 \rightarrow 1$ later on]. "Temperatures" are introduced via a substitution: $\mathcal{Q} \Rightarrow \mathcal{Q}T$.

• Consider the process

$$\ddot{x} = \phi \rightarrow \begin{cases} \dot{v} = T_1 \phi_1 \\ \dot{x} - v = T_2 \phi_2 \end{cases} \quad (1.2.64)$$

Then:

$$W^{T_1 T_2}(x_1 v_1 + | x_0 v_0, 0) = \int_{C[x_0 v_0, 0; x_1 v_1, t]} \prod \frac{dv(\tau)}{\sqrt{\pi T_1 d\tau}} \prod \frac{dx(\tau)}{\sqrt{\pi T_2 d\tau}} \times$$

$$\times \exp \{ - (?) \} \quad (1.2.65)$$

This is the case of "interacting" two particles considered above:

$$\begin{cases} \dot{x}_1 + k_{11}x_1 + k_{12}x_2 = \phi_1 \\ \dot{x}_2 + k_{21}x_1 + k_{22}x_2 = \phi_2 \end{cases} \rightarrow k = \begin{pmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}$$

with $\text{Tr} k = 0 \rightarrow \text{Jacobian} = 1$. Then, we only have

$$(?) = \frac{1}{T_1} \int_0^t \dot{v}^2 ds + \frac{1}{T_2} \int_0^t (\dot{x} - v)^2 ds$$

in the exponential.

• Use the discrete time approximation for a part of the integral:

$$\prod \frac{1}{\sqrt{\pi \delta\tau T_2}} \exp \left(- \frac{1}{T_2} \int_0^t (\dot{x} - v)^2 ds \right)$$

$$\hookrightarrow \prod_{i=0}^N \frac{1}{\sqrt{\pi \varepsilon T_2}} \cdot \exp \left[- \frac{1}{T_2} \sum_{j=0}^N \left(\frac{x_{j+1} - x_j}{\varepsilon} - v_j \right)^2 \varepsilon \right]$$

$$= \prod_{i=0}^N \left(\frac{1}{\sqrt{\pi \varepsilon T_2}} \exp \left[- \frac{1}{T_2} \left(\frac{x_{j+1} - x_j}{\varepsilon} - v_j \right)^2 \varepsilon \right] \right)$$

We know:

$$\delta(x) = \lim_{\alpha \rightarrow \infty} \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2 x^2}$$

$$\text{or, if } T = 1/\alpha^2 \rightarrow \delta(x) = \lim_{T \rightarrow 0} \frac{1}{\sqrt{\pi T}} e^{-x^2/T}$$

so that in the $T_2 \rightarrow 0$ limit we get

$$\prod_{i=0}^N \frac{1}{\sqrt{\epsilon}} \delta \left[\left(\frac{x_{j+1} - x_j}{\epsilon} - v_j \right) \sqrt{\epsilon} \right] = \prod_{i=0}^N \frac{1}{\epsilon} \delta \left(\frac{x_{j+1} - x_j}{\epsilon} - v_j \right)$$

$$= \prod_{\tau=0}^t \frac{1}{\epsilon} \delta(\dot{x}(\tau) - v(\tau)) = \underbrace{\frac{1}{\epsilon^N} \delta[\dot{x}(\tau) - v(\tau)]}_{\text{product of } \delta\text{-f. at each slice of time}} \prod_{\tau=0}^t \frac{1}{\epsilon} d\tau$$

Insert into (1.2.65) [$T_1 \rightarrow 1$ here], while considering the $dx(\tau)$

~~$$W(x_t, v_t | x_0, v_0) = \int \prod_{\tau=0}^t \frac{dv(\tau)}{\sqrt{\pi}} \cdot \prod_{\tau=0}^t \frac{dx(\tau)}{\sqrt{\pi}} \exp \left[- \int_0^t d\tau \dot{x}^2 \right] \times$$

$$\times \delta[\dot{x}(\tau) - v(\tau)]$$~~

integral in the discretised way:

$$\int \frac{dx(\tau)}{\sqrt{\pi}} \dots \rightarrow \prod_{i=0}^N \int \frac{dx_1}{\epsilon} \int \frac{dx_2}{\epsilon} \dots \int \frac{dx_N}{\epsilon} \prod_{j=0}^N \delta \left(\frac{x_{j+1} - x_j}{\epsilon} - v_j \right)$$

$$= \int dx_1 \int dx_2 \dots \int dx_N \prod_{j=0}^N \delta(x_{j+1} - x_j - v_j \epsilon)$$

$$= \int dx_1 \dots \int dx_N \delta(x_1 - x_0 - v_0 \epsilon) \delta(x_2 - x_1 - v_1 \epsilon) \dots \delta(x_N - x_{N-1} - v_{N-1} \epsilon) \times$$

$$\times \delta(\underbrace{x_{N+1}}_{x_t} - x_N - v_N \epsilon) = \int dx_1 \dots \int dx_{N-1} \delta(x_1 - x_0 - v_0 \epsilon) \times \dots \times \delta(x_{N-1} - x_{N-2} - v_{N-2} \epsilon)$$

$$\times \delta(x_t - v_N \epsilon - x_{N-1} - v_{N-1} \epsilon) =$$

$$= \int dx_1 \dots \int dx_{N-2} \dots \delta(x_{N-3} - x_{N-2} - v_{N-3} \epsilon) \delta(x_{N-2} - x_{N-3} - v_{N-2} \epsilon) \times$$

$$\times \delta(x_t - x_{N-2} - (v_{N-2} + v_{N-1} + v_N) \epsilon) = \dots =$$

$$= \int dx_1 \delta[x_t - x_0 - (v_0 + v_1 + \dots + v_N) \epsilon] = \delta \left(x_t - x_0 - \int_0^t v(\tau) d\tau \right)$$

This finally gives:

$$W(x_t, v_t, t | x_0, v_0, 0) = \int_{C[v_0, 0; v_t, t]} d_w v(\tau) \delta\left(x(t) - x(0) - \int_0^t v(\tau) d\tau\right) \prod_{\tau=0}^t \frac{dv(\tau)}{\sqrt{\pi d\tau}} \exp\left(-\int_0^t \dot{v}(\tau)^2 d\tau\right)$$

1.2.5. Bloch eq. and Feynman-Kac formula

(1.2.70)

- Bloch eq. lactides can be removed (annihilated) with probability $V(x, t)$ per unit time. Then

$$\underbrace{\bar{J} = -D \frac{\partial \rho}{\partial x}}_{\text{current}} \quad \text{and} \quad \underbrace{\frac{\partial \rho}{\partial t}}_{\text{change of } \rho} = \underbrace{-\frac{\partial \bar{J}}{\partial x}}_{\text{reduced due to current}} - \underbrace{V\rho}_{\text{reduced due to annihilation}} \Rightarrow \boxed{\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2} - V\rho} \quad (1.2.76)$$

For Via the path integral:

$$W_D(x_t, t | x_0, t_0) = \int_{C[x_0, t_0; x_t, t]} d_w x(\tau) \exp\left[-\int_0^t V(x, s) ds\right] \quad (1.2.79)$$

probability to remain on the trajectory up to time t

- $t > t_0$ condition can be imposed by putting $\Theta(t-t_0)$ in front:

$$W'_D(x, t | x_0, t_0) = \Theta(t-t_0) W_D(x, t | x_0, t_0)$$

where

W_D satisfies usual diffusion eq:

$$\left(\frac{\partial}{\partial t} - D \frac{\partial^2}{\partial x^2}\right) W'_D = \underbrace{\Theta(t-t_0) \left(\frac{\partial}{\partial t} - D \frac{\partial^2}{\partial x^2}\right) W_D}_0 + \delta(t-t_0) \underbrace{W_D(x, t | x_0, t_0)}_{\rightarrow \delta(x-x_0) \text{ when } t \rightarrow t_0}$$