III. General form of Langevin equations

so far we had equations of the form

$$\dot{\underline{v}} = -\gamma \underline{v} + m^{-1} \underline{f}(t)$$

Generalization:

let $\{\underline{x}(t)\} = x_1(t), x_2(t), \ldots, x_M(t)$
be a set of dynamical variables

$$(*) \qquad \boxed{\dot{x}_i(t) = h_i(\{\underline{x}(t)\}, t) + \sum_{j=1}^{M} D_{ij}(\{\underline{x}(t)\}, t) f_j(t)}$$

where $\langle f_i \rangle = 0$

$\langle f_i(t) f_j(t') \rangle = \Gamma_i \delta_{ij} \delta(t-t')$

$D_{ij} = \text{const}$ „additive noise"

D_{ij} depends on $\underline{x}$: „multiplicative noise" sometimes one needs the integral form of the equation (+)

$$\Rightarrow x_i(t+\tau) - x_i(t)$$

$$= \int_t^{t+\tau} dt' \, h_i(\{\underline{x}_i(t')\}, t')$$

$$+ \int_t^{t+\tau} dt' \sum_{j=1}^{M} D_{ij}(\{\underline{x}_i(t')\}, t') \, f_j(t') \qquad (**)$$

notice the (possible) problem in the second term:

$f_j(t')$ is highly irregular (random variable with zero correlation time!)
this irregularity transfers to $\underline{x}(t)$

$\Rightarrow$ which value of $f_j(t')$ and $\underline{x}(t')$ shall we use to evaluate the integral?

note: This problem does not occur for the first term since h_i is assumed to be a deterministic, regular function

$\Rightarrow$ we can just approximate

$$\int_t^{t+\tau} dt' \, h_i(\{\underline{x}(t')\}, t') \longrightarrow h_i(\{\underline{x}(t')\}, t') \cdot \tau$$

for small τ

$\Rightarrow$ Problem of stochastic integrals!

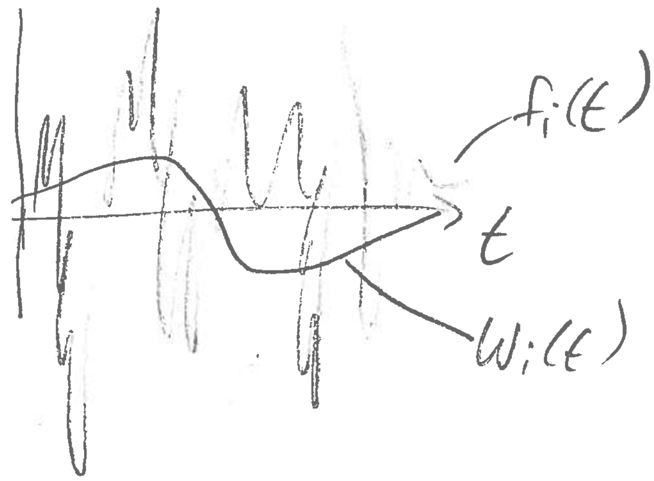
strategy:

introduce the "Wiener increment"

$$W_i(\tilde{\tau}) = \int_t^{t+\tilde{\tau}} dt' \, f_i(t')$$

$$dW_i(t) = f_i(t)\, dt$$

note : W_i behaves somewhat smoother than f_i



but : $\dot{W}_i = f_i(t)$ does not exist, strictly speaking!

insert into (**):

$$x_i(t+\tilde{\tau}) - x_i(t) = \int_t^{t+\tilde{\tau}} dt' \, h_i(\{\underline{x}(t')\}, t') + \int_t^{t+\tilde{\tau}} \sum_{j=1}^{M} D_{ij}(\{\underline{x}(t')\}, t')\, dW_j(t')$$

("Riemann - Stieltjes integral")

note: there are two ways to evaluate the stochastic integral in the second term!

1) Ito
2) Stratonovich

Consider integrals of the type (one-dimensional) $A = \int_t^{t+\tau} D(x(t'), t')\, dW(t')$

Discretization: Divide the time interval τ into N sub-intervals

$$A^{Ito} = \lim_{N\to\infty} \sum_{m=0}^{N} D(x(t_m), t_m)\left(W(t_{m+1}) - W(t_m)\right)$$

$\Rightarrow$ evaluation of D at the left boundary of each subinterval

$$A^{Stratonovich} = \lim_{N\to\infty} \sum_{m=0}^{N} \left[\tfrac{1}{2}\left(D(x(t_{m+1}), t_{m+1}) - D(x(t_m), t_m)\right) \cdot \left(W(t_{m+1}) - W(t_m)\right)\right]$$

$\Rightarrow$ evaluation via an average of D!

Note: For $D = \text{const}$ we have $A^{Ito} = A^{Stratonovich}$!!

Where is this issue important ??

E.g., for the relation between Langevin-like equations and the Fokker-Planck equation!

Consider the so-called <u>Kramers-Moyal coefficients</u>

$$K^{(n)}_{i_1 i_2 \ldots i_n}(\{\underline{x}(t)\},t) = \frac{1}{n!}\lim_{\tau\to 0}\frac{1}{\tau}\Big\langle (x_{i_1}(t+\tau)-x_{i_1}(t)) \cdot (x_{i_2}(t+\tau)-x_{i_2}(t)) \cdots (x_{i_n}(t+\tau)-x_{i_n}(t))\Big\rangle\Big|_{\text{fixed } \{\underline{x}(t)\}}$$

Strategy to calculate the $K^{(n)}$'s:

use $\quad x_i(t+\tau)-x_i(t) = \int_t^{t+\tau} dt' \left[h_i(\{\underline{x}(t)\},t) + \sum_j D_{ij}(\{\underline{x}(t)\},t')\, f_j(t') \right]$

$(i=1,..,M)$

and expand the functions h_i and D_{ij} around the (fixed) vector $\underline{x}(t)$

The averages $\langle \ldots \rangle$ can then be calculated as time averages result:

$$K_i^{(1)} = \lim_{\tau \to 0} \frac{1}{\tau} \langle x_i(t+\tau) - x_i(t) \rangle$$

$$\boxed{\begin{aligned} K_i^{(1)} &= h_i(\{\underline{x}(t)\}, t) \\ &+ \frac{\Pi}{2} \sum_{jk} \frac{\partial D_{ij}}{\partial x_k}(\{\underline{x}(t)\}, t) D_{kj}(\{\underline{x}(t)\}, t) \end{aligned}} \quad (*)$$

so-called "drift coefficient"

Note:

- The second term in (*) is the so-called 'noise-induced' drift.
  It arises only in the Stratonovitch interpretation, not for Ito !!

- The noise-induced drift vanishes anyway if $D_{ij} = \text{const}$

- Example (simple Brownian motion)

$$\left.\begin{aligned} \dot{r} &= v \\ \dot{v} &= -\gamma v + m^{-1} f(t) \end{aligned}\right\} \Rightarrow \begin{aligned} & h_r = 0 \quad , h_v = -\gamma v \\ & D_{rr} = D_{rv} = D_{vr} = 0 \\ & D_{vv} = +\frac{1}{m} \end{aligned}$$

$$\Rightarrow K_r^{(1)} = 0$$

$$K_v^{(1)} = -\gamma v$$

Second Kramers-Moyal coefficient

$$K^{(2)}_{ij}(\{\underline{x}(t)\},t)$$
$$= \frac{1}{2}\lim_{\tau\to 0}\frac{1}{\tau}\langle (x_i(t+\tau)-x_i(t))(x_j(t+\tau)-x_j(t))\rangle$$

one finds:

$$\boxed{K^{(2)}_{ij} = \frac{\Pi}{2}\sum_k D_{ik}(\{\underline{x}(t)\},t)\,D_{kl}(\{\underline{x}(t)\},t)}$$

often called "diffusion coefficient" (in a generalized sense !!)

also note:

if the stochastic forces are distributed via a Gauss distribution,

$$\boxed{K^{(n)}_{i_1 i_2 \ldots i_n} = 0 \quad \text{for } n \geq 3} \quad !!$$

Examples for $K^{(2)}$: non-overdamped Brownian particle

$$\dot{r} = v$$
$$\dot{v} = -\gamma v + m^{-1} f(t)$$

$$D_{rr} = D_{rv} = D_{vr} = 0$$
$$D_{vv} = \frac{1}{m}$$

we already had: $K_v^{(1)} = -\gamma v$!

$$\Rightarrow K_{vv}^{(2)} = K^{(2)} = \frac{\Gamma}{2m^2}$$

$$= \gamma \frac{k_B T}{m} = \gamma^2 D$$

equilibrium (equipartition)

Einstein

overdamped case:

$$-\gamma v = m^{-1} f(t)$$
$$v = -\frac{1}{\gamma m} f(t) \quad \Rightarrow h_v = 0, \; D_{vv} = \left(-\frac{1}{\gamma m}\right)$$

$$\Rightarrow K_v^{(1)} = 0$$
$$K_{vv}^{(2)} = \frac{\Gamma}{2}\left(+\frac{1}{\gamma^2 m^2}\right) = \gamma k_B T m \cdot \frac{1}{\gamma^2 m^2} = \frac{k_B T}{\gamma m} = \underline{\underline{D}}$$

normal diffusion coefficient!

IV. Fokker-Planck equation

starting point:

Master equation (for continuous variables, here in 1D)

$$\frac{\partial}{\partial t} P(x,t) = \int dx' \Big[\underbrace{W(x;x't)\, P(x',t)}_{\text{gain}} \\ \underbrace{- W(x';x t)\, P(x,t)}_{\text{loss}} \Big]$$

$\Rightarrow$ strictly speaking, one needs to know the transition rates over the entire space ($\int dx'$) !

we now assume that the transition rates are significant only if x' is close to x

$\Rightarrow$ expand the transition rates in powers of $\Delta = x - x'$

„Kramers-Moyal expansion"

(here we will not do this expansion explicitely ...)

Result:

$$\boxed{\frac{\partial}{\partial t} P(x,t) = \sum_{n\geq 1}^{\infty} \left(-\frac{\partial}{\partial x}\right)^n \tilde{K}^{(n)}(x,t)\, P(x,t)} \quad (*)$$

where $\tilde{K}^{(n)}(x,t) = \frac{1}{n!} \int_{-\infty}^{\infty} d\Delta \, (\Delta)^n \, W(x+\Delta; x,t)$

Note:
One can further show that $\tilde{K}^{(n)}(x,t)$ is identical to the Kramers-Moyal coefficient defined in Chapter III !!

i.e. $\tilde{K}^{(n)}(x,t) = K^{(n)}(x,t)$

$$= \frac{1}{n!} \lim_{\tau \to 0} \frac{1}{\tau} \langle (x(t+\tau) - x(t))^n \rangle$$

Specialize now to the case that only

$K^{(1)} \neq 0$, $K^{(2)} \neq 0$, but $K^{(n)} = 0$ for $n \geq 3$

exactly valid for Gaussian random forces

(more generally: $K^{n\geq 3} \approx 0$ for systems where the transition probability strongly decays ...)

$$\Rightarrow \frac{\partial}{\partial t} P(x,t) = \left[-\frac{\partial}{\partial x} K^{(1)}(x,t) + \frac{\partial^2}{\partial x^2} K^{(2)}(x,t) \right] P(x,t)$$

note: The partial derivatives act both on $K^{(1)}, K^{(2)}$ and on $P(x,t)$!!

many variables:

$$\boxed{\frac{\partial}{\partial t} P(\{\underline{x}\},t) = \left[-\sum_{i=1}^{M} \frac{\partial}{\partial x_i} K_i^{(1)}(\{\underline{x}\},t) + \sum_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} K_{ij}^{(2)}(\{\underline{x}\},t) \right] P(\{\underline{x}\},t)}$$

Fokker-Planck equation (FP)

e.g. Brownian particle, non-overdamped, with external force $F(x)$
$x_1 = x$
$x_2 = y$
$x_3 = z$
$x_4 = v_x$
$x_5 = v_y$
$x_6 = v_z$

<u>note</u>:

- The expression $[\ldots]$ is the FP operator

$$\frac{\partial}{\partial t} P = \hat{L}_{FP} P$$

- Rewrite the FP equation as continuity equation

define current: $J_i = K_i^{(1)} P - \sum_j \frac{\partial}{\partial x_j} K_{ij}^{(2)} P$

$\longrightarrow$

$$\Rightarrow \boxed{\frac{\partial}{\partial t} P(\{\underline{x}\},t) + \underbrace{\sum_i \frac{\partial}{\partial x_i} J_i}_{\text{"}\nabla\cdot\underline{J}\text{"}} = 0}$$

expresses conservation of the ~~total~~ probability!

$$\int d\underline{x} \; P(\{\underline{x}\},t) = 1$$

stationary process:

$$\frac{\partial}{\partial t} P(\{\underline{x}\},t) = 0$$

$$\Leftrightarrow \underline{J} = \text{const}$$

Stationary solution of the FP equation

consider, for simplicity, a problem in 1D

(e.g. overdamped Brownian particle in 1D)

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

$$\text{where } J(x,t) = \left(K^{(1)}(x) - \frac{\partial}{\partial x} K^{(2)}(x) \right) P(x,t)$$

~~stationary~~ equilibrium state $\Rightarrow J = 0$ and $P(x,t) \Rightarrow P^{\cancel{stat}\,eq}(x)$

$$\underbrace{K^{(1)}(x)\, P^{\cancel{stat}\,eq}(x)} = +\frac{\partial}{\partial x}\left(K^{(2)}(x)\, P^{\cancel{stat}\,eq}(x) \right)$$

$$\frac{K^{(1)}(x)}{K^{(2)}(x)}\, K^{(2)}(x) P^{\cancel{stat}\,eq}(x) = \frac{\partial}{\partial x}\left(K^{(2)}(x) P^{\cancel{stat}\,eq}(x) \right)$$

$$\Rightarrow K^{(2)}(x) P^{\cancel{stat}\,eq}(x) = \alpha\, e^{\int_c^x dx' \frac{K^{(1)}(x')}{K^{(2)}(x')}}$$

$$\Rightarrow P^{\cancel{stat}\,eq}(x) = \frac{\alpha}{K^{(2)}(x)}\, e^{\int_c^x dx' \frac{K^{(1)}(x')}{K^{(2)}(x')}}$$

$$\equiv \alpha\, e^{-\phi(x)}$$

c is an (irrelevant) integration constant

$$\text{where } \phi(x) = \ln K^{(2)}(x) - \int_c^x dx' \frac{K^{(1)}(x')}{K^{(2)}(x')}$$

one sees: $K^{(2)}$ must be positive !!

e.g. non-overdamped Brownian particle, no external forces, 1D

$x \to v$

$K^{(1)} = -\gamma v \,, \quad K^{(2)} = m^{-2}\frac{\Gamma}{2}$

one finds: $$\Phi(v) = \ln\frac{\Gamma}{2} - \int_0^v dv' \, \frac{(-\gamma v')}{\Gamma/2 \, m^{-2}}$$

$$= \ldots = \text{const} + \underbrace{\frac{\gamma m^2}{\Gamma}}_{\frac{m}{2 k_B T}} v^2$$

$$\Rightarrow P^{stat}(v) \sim e^{-\frac{m}{2k_BT} v^2}$$

Maxwell-Boltzmann distribution

as expected !!

$\Rightarrow \frac{\partial}{\partial t} P(x,t) \approx 0$

$\rightarrow J(x,t) \approx \text{const} = J$

current density

constant in space and time!!

("quasi-stationary state")

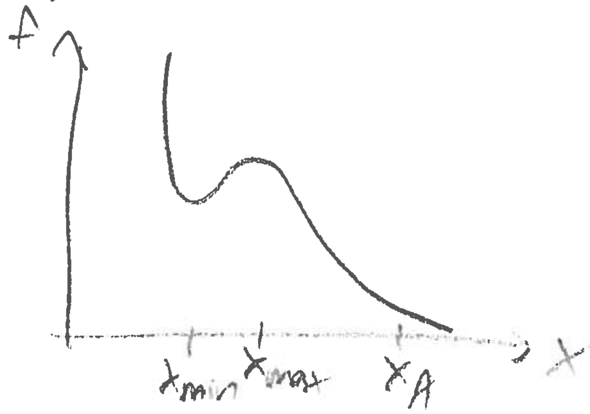
$\Rightarrow$ from (*):

$$J e^{f(x)/D} = -D \frac{\partial}{\partial x}\left(e^{f(x)/D} \underline{P(x)}\right)$$

assumed to be independent of t!

integrate from x_{min} to a point x_A outside the barrier

- and assume that $P(x_A) \approx 0$, since the particles are essentially trapped in the valley!!



$$\Rightarrow J = D e^{f(x_{min})/D} \cdot P(x_{min}) \cdot \left[\int_{x_{min}}^{x_A} dx' e^{f(x')/D}\right]^{-1}$$

Consider now the <u>probability density</u>:

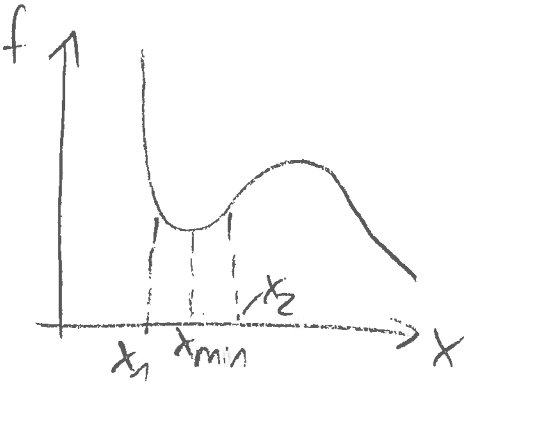
note: We have already assumed that we can work in the stationary limit !!

$$\Rightarrow P(x) \rightarrow P^{stat}(x) = e^{-\Phi(x)}$$

where $\Phi(x) = f(x)/D$

$$\Rightarrow \frac{P(x)}{P(x_{min})} = e^{-[f(x)-f(x_{min})]/D}$$ for any point x in the valley

integrate to get the total probability to find the particle within the valley



$$\rho = \int_{x_1}^{x_2} dx\, P(x)$$

$$= P(x_{min})\, e^{f(x_{min})/D} \int_{x_1}^{x_2} dx\, e^{-f(x)/D}$$

Combine this with our result for the current: