Classical Mechanics Recap

Hamilton

$$H(v, r; t) = \underset{= \frac{1}{2}mv^2}{K} + V$$

$$\frac{\partial v}{\partial t} = \frac{1}{m}\underbrace{\left(-\frac{\partial V}{\partial r}\right)}$$

$$= \frac{1}{m} f \quad (+\text{ non-gradient forces})$$

$$\frac{\partial r}{\partial t} = v$$

conservation of phase space $\rho_\Omega(x) = \rho_{\tilde{\Omega}}(\tilde{x})$

$$\tilde{x} = g(x)$$

Transform $\rho_{\tilde{\Omega}}(\tilde{x}) = \rho_{\Omega}(g^{-1}(\tilde{x})) \left| \frac{d}{dx} g^{-1}(x) \right|$

Liouvillian

$$\frac{\partial \rho}{\partial t} = -\mathcal{L}\rho$$

Liouvillian

$$\rho = e^{-\Delta t \mathcal{L}}$$

Lagrangian

$L = K - V$

Action $A = \int_{t_1}^{t_2} L \, dt$

principle of least action

②

ξ Xi "Zai"

Langevin Dynamics

underdamped

$$\frac{dx}{dt} = v$$

friction

Random force

$$\underbrace{m\frac{dv}{dt}}_{a} = \underline{f}(x) - \gamma v + \xi(t)$$

$$\langle \xi(t) \rangle = 0 \qquad \langle \xi(0)\,\xi(t) \rangle = \frac{2\gamma}{\beta}\,\delta(t)$$

(Linear Response)

High friction

$$0 = f(x) - \gamma\frac{dx}{dt} + \xi(t), \qquad \gamma\frac{dx}{dt} = f(x) + \xi(t)$$

FT Theorem

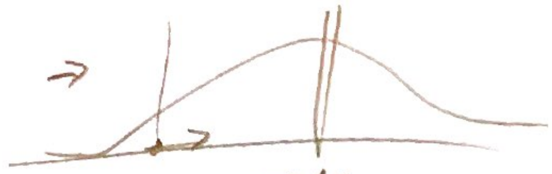
$\langle e^{-\Sigma} \rangle = 1$ Gaussian $P(\Sigma) = \dfrac{e^{-\frac{(\Sigma-\langle\Sigma\rangle)^2}{2\sigma^2}}}{\sqrt{2\pi\sigma^2}}$ $\ln\langle e^{+\alpha\Sigma}\rangle = \alpha\langle\Sigma\rangle + \dfrac{\alpha^2}{2}\sigma_\Sigma^2$

$\alpha = -1$ $\langle\Sigma\rangle = \dfrac{\sigma^2}{2}$

Linear Response

Fluctuation-dissipation theorem $\beta\langle w\rangle = \dfrac{\beta^2\sigma_w^2}{2}$

Impose const force



$$\gamma \frac{dx}{dt} = f(x) + \xi(t)$$

$\langle v\rangle = \dfrac{f}{\gamma}$ $\sigma_{\Delta x}^2 = \dfrac{\Delta t}{\gamma^2}\sigma_\xi^2$

$\langle \Delta x\rangle = \Delta t\langle v\rangle = \dfrac{\Delta t f}{\gamma}$ $\sigma_w^2 = \sigma_{\Delta x f}^2 = f^2\sigma_{\Delta x}^2 = \dfrac{f^2}{\gamma^2}\Delta t\,\sigma_\xi^2$

$\langle w\rangle = \Delta t\dfrac{f^2}{\gamma}$ $\sigma_w^2 = \dfrac{2}{\beta}\dfrac{\Delta t f^2}{\gamma} = \dfrac{f^2\Delta t}{\gamma^2}\sigma_\xi^2$ $\boxed{\sigma_\xi^2 = \dfrac{2\gamma}{\beta}}$

Einstein Relation

$$D = \lim_{\Delta t \to \infty} \frac{\langle \Delta x^2 \rangle}{2 \Delta t} = \frac{\mu}{\beta}$$

mobility $= \frac{\langle v \rangle}{F} = \gamma$

$$D = \frac{2\gamma}{\beta\, 2} = \frac{\gamma}{\beta}$$

← friction coefficient or mobility

Stieltjes Integral $\int f(x)\, dg(x) = \int f(x)\, g'(x)\, dx$

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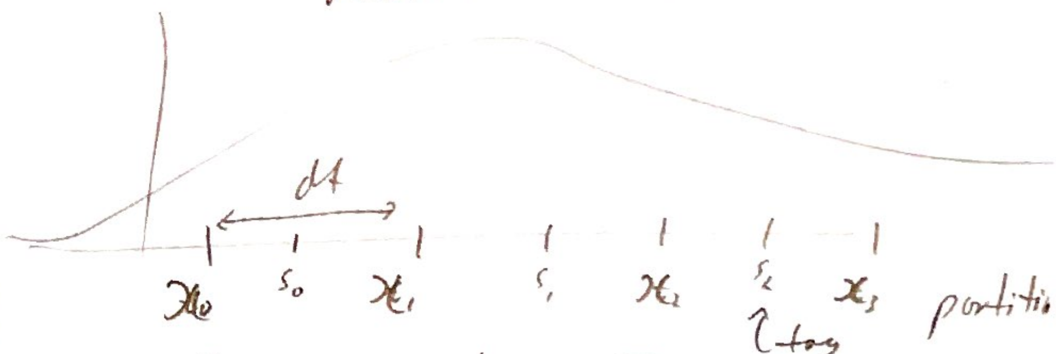
Stocastic Calculus

$W(t)$ }  } Random walk, zero mean

Weiner process

$$\int_a^b dt\, \xi(t)\, f(t) = \int dW(t)\, f(t)$$

Reimann integral



Reimann sum $\lim_{dt \to 0} \sum f(s_i)(x_{i+1} - x_i)$

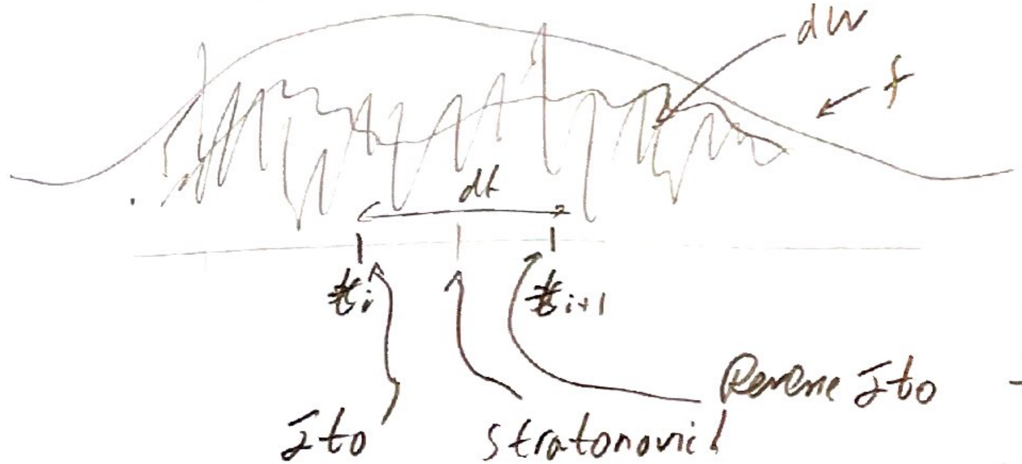
But For Regular integrals ("well behaved") where tag is doesn't matter

But Does for Stocastic Integrals

* MoAL 4 Econonics → Ito

* Much of (but not all) of physics → Stratonovich

Bi linear.



Ito

$$I_I = \lim_{dt \to 0} \sum [W(t_{i+1}) - W(t_i)] f(t_i)$$

Chain Rule different
Not time symmetric

Stratonovich

$$I_S = \lim_{dt = 0} \sum [W(t_{i+1}) - W(t_i)) f\left(\frac{t_i + t_{i+1}}{2}\right)$$

$(S) \int_a^b dW f(t)$

Regular chain Rule
time symmetric

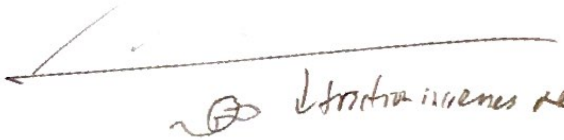
Stratonovich

$$\int_c^d dW \circ f(t)$$

$$\frac{d[f(x)]}{dt} = f'(x) \frac{dx}{dt}$$

Reverse Ito

$$I_R = \lim_{dt \to 0} \sum [W(t_{i+1}) - W(t_i)) f(t_{i+1})$$



↓ friction increases near wall

$$m \frac{\partial v}{\partial t} = f(x,t) - \gamma(x,t) + \xi(t)$$

If friction coordinate dependent
then Ito ≠ Stratonovich.

"spurious forces"

$$D = \frac{\gamma}{\beta}$$

Fokker Planck Equation $\equiv$ Master Equation for Brownian Motion

ITO !

$$\frac{d}{\partial t} p = -\frac{\partial}{\partial x} f(x,t)\, p(x,t) + \frac{1}{\beta}\frac{\partial^2}{\partial x^2}\left[\cancel{\gamma}(x,t)\, p(x,t)\right]$$

stratonovich

$$= + \frac{1}{\beta}\frac{\partial}{\partial x}\left[\gamma(x,t)\, \frac{\partial}{\partial x} p(x,t)\right]$$

same if $\gamma(x,t)$ not position dependent

$S \Rightarrow$ "spurious forces"

$\gamma \ell \leftarrow$ Maintains detailed balance

~~Fokker - Planck Equation~~

$$\frac{\partial}{\partial t}\rho = -\mathcal{L}\rho \qquad \mathcal{L} = \mathcal{L}_c + \mathcal{L}_{OU}$$

Liouvillian

$$= \mathcal{L}_V + \mathcal{L}_R$$

$$\frac{f}{m}\frac{\partial}{\partial v} \qquad v\frac{\partial}{\partial r} \qquad -\gamma\frac{\partial}{\partial v}v - \frac{\gamma^2}{\beta m}\frac{\partial^2}{\partial v^2}$$

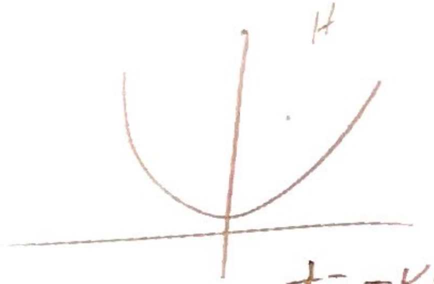
Ornstein-Uhlenbeck Process
(on velocities)

$$\rho(\Delta t)\ e^{-\Delta t \mathcal{L}}\ \rho(t)$$

$$e^{-\Delta t \mathcal{L}} = e^{-\Delta t(\mathcal{L}_V + \mathcal{L}_R + \mathcal{L}_O)}$$

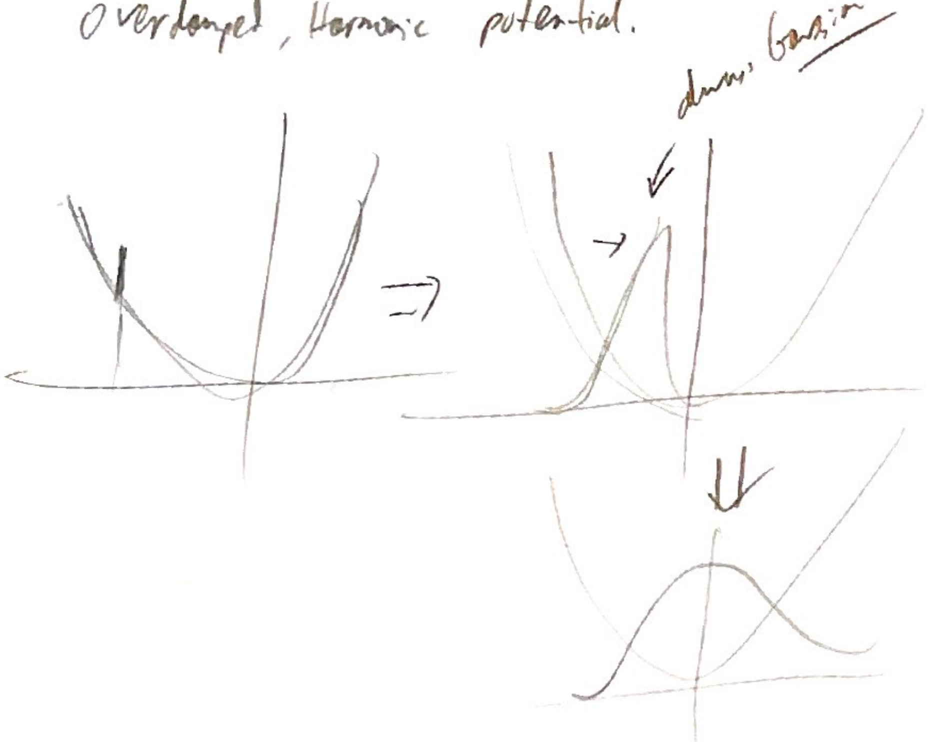
Ornstein-Uhlenbeck (OU) Process

$$\gamma \frac{dx}{dt} = -Kx + \xi$$



$f = -Kx$

Overdamped, Harmonic potential.



$$\frac{\partial \rho}{\partial t} = -\mathcal{L}\rho$$ "Fokker Plank equation"

$$\mathcal{L} = -K\frac{\partial}{\partial x}x - \frac{\gamma^2}{\beta m}\frac{\partial^2}{\partial x^2}$$

Diffusion equation in Harmonic potential

$e^{\epsilon(A+B+C)} \approx e^{\epsilon A/2} e^{\epsilon B/2} e^{\epsilon C/2} e^{\epsilon C/2} e^{\epsilon B/2} e^{\epsilon A/2}$

Ben Leimkuhler 2013

BAOAB

$O = e^{-\frac{\Delta t}{2}\mathcal{L}_O}$ OVRRVO velocity verlet RVOOVR

$R = e^{-\frac{\Delta t}{2}\mathcal{L}_R}$ ORVVRO VROORV

$V = e^{-\frac{\Delta t}{2}\mathcal{L}_V}$ ROVVOR × VORROV ×

$V(t+1/2) = \sqrt{a}\,v(t) + \sqrt{\frac{1-a}{\beta m}}\,N$ ← Normal.

$a = e^{-\gamma \Delta t}$

(Heat & Work!)

shadow work.