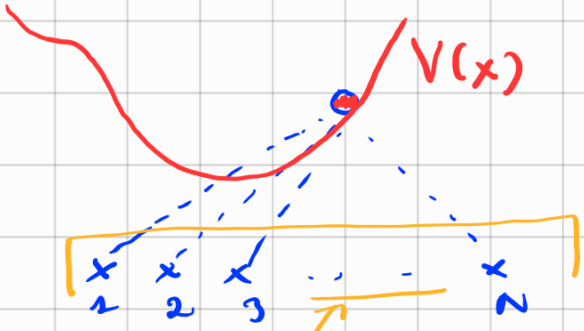
# One particle interacting with $N (\to \infty)$ harmonic oscillators

From reversible to dissipative dynamics




Noise → $\xi(t)$

Friction → $\gamma(t-t')$

$$M\ddot{X} = -\frac{\partial \tilde{V}}{\partial X} + \xi(t) - M\int_0^t dt'\, \gamma(t-t')\, \dot{X}(t')$$

Generalised Langevin

$\xi(t) = \sum_\lambda c_\lambda y_\lambda^{(0)}(t)$ ← interaction constants

params $\{c_\lambda, m_\lambda, \omega_\lambda\}$

$N \to \infty$ → statistical properties of noise

→ specify distributions

→ coupling

→ frequencies

## Spectral Density (Ohmic)

inverse correlation time $\Gamma^2$

$$J(\omega) = \frac{\pi}{2}\sum_\lambda \frac{c_\lambda^2}{m_\lambda \omega_\lambda}\,\delta(\omega-\omega_\lambda) \underset{N\to\infty}{=} M\gamma\,\frac{\omega\,\Gamma^2}{\omega^2+\Gamma^2}$$

$N \to \infty$

Coupling

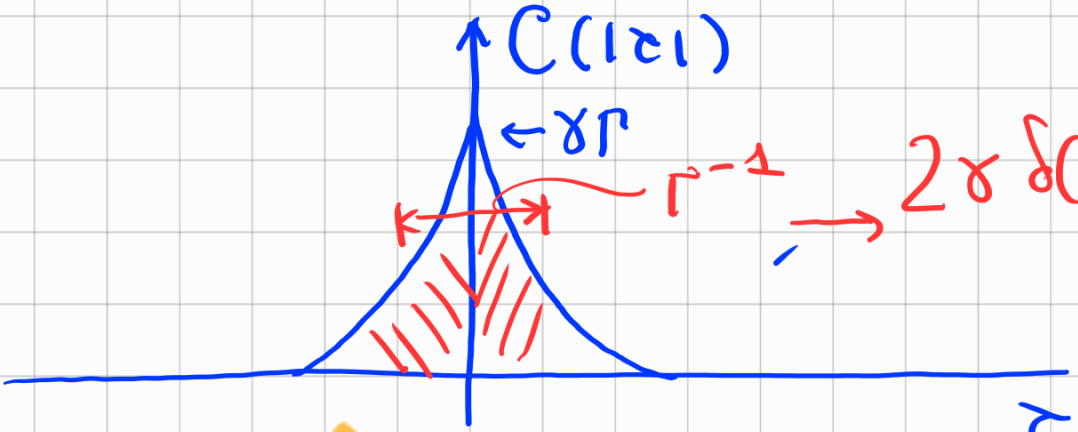
$$\langle \xi_\epsilon(t) \rangle = 0$$

$$\langle \xi_\epsilon(t)\,\xi_\epsilon(t') \rangle = \frac{M}{\beta}\,\gamma(|t-t'|)$$

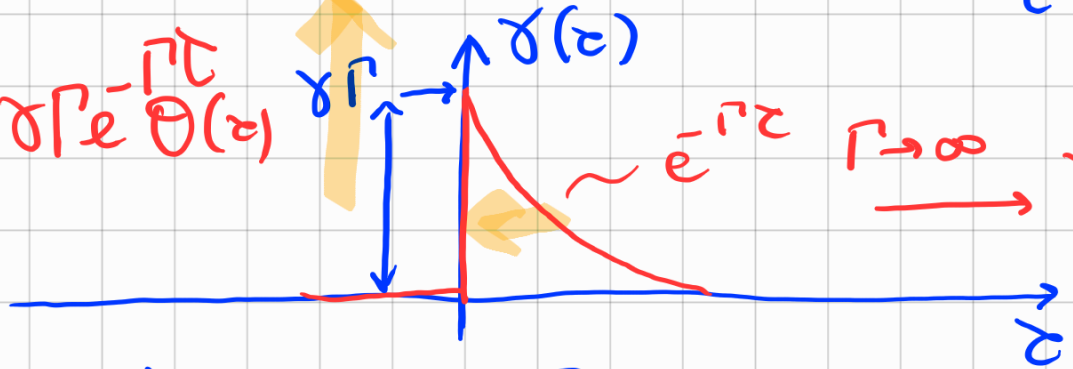
$$\gamma(t) = \theta(t)\,\gamma\Gamma e^{-\Gamma t}$$

$\Gamma^{-1}$ $\Rightarrow$ decorrelation time of the noise

$$\langle \xi(t)\,\xi(t') \rangle = C(\underbrace{|t-t'|}_{\tau})$$




$$\gamma(\tau) = \gamma\Gamma e^{-\Gamma\tau}\,\theta(\tau)$$




White Noise Limit $\Gamma \to \infty$

# Langevin Equation

noise

$$\dot{P} = -\frac{\partial \tilde{V}}{\partial x} + \xi(t) - \gamma P$$

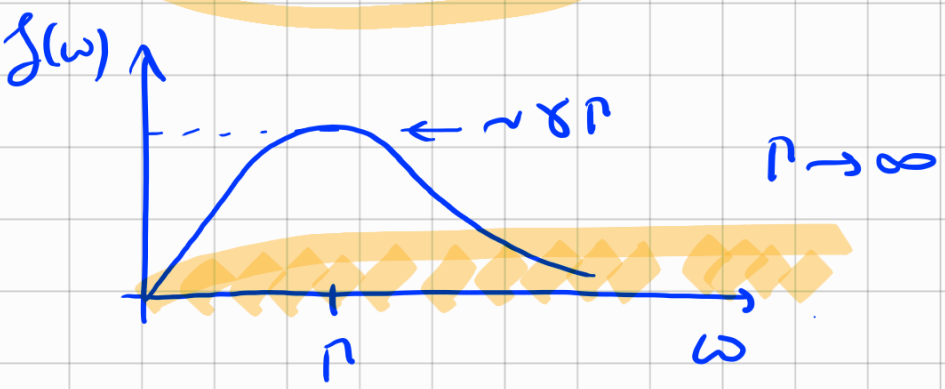
friction

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

$$\langle \xi(t)\xi(t') \rangle = 2\frac{M\gamma}{\beta}\delta(t-t')$$

Hamiltonian $H = H_S + H_B + H_{SB}$ reversible dynamics

## $N \to \infty$ limit



1) Langevin Equation

↳ Drift under external force **DISSIPATION**

↳ fluctuations, diffusion in absence of ext force **FLUCTS**

2) Langevin eq → goes to Maxwell Boltzmann eq wlibrium

**Free particle under external (time dep ...) Force**

(DRIFT)

$$\dot{p} = -\gamma p + \xi(t) + F(t)$$

$\xi(t)$: random

$F(t)$: constant (x independent)

average momenta

$$\langle p(t) \rangle$$

$$\langle \dot{p} \rangle = -\gamma \langle p \rangle + \cancel{\langle \xi(t) \rangle} + F$$

$$\frac{d\langle p(t) \rangle}{dt} = -\gamma \langle p(t) \rangle + F$$

for large times and constant $F$

$$\lim_{t \to \infty} \langle p(t) \rangle = \langle p \rangle$$

$$0 = -\gamma \langle p \rangle + F$$

$$\boxed{\langle p \rangle = \frac{F}{\gamma}}$$

Aristotle law of motion

Conductivity

$\vec{J} = \rho \langle \vec{v} \rangle$ $\quad \vec{F} = e\vec{E}$

$\rho$: charge density $= e\rho_m$ ($e$: charge, $\rho_m$: number density)

$$\langle \vec{v} \rangle = \frac{\vec{F}}{M\gamma}$$

$$\vec{J} = \left(\frac{e^2 \rho_m}{M\gamma}\right)\vec{E} \qquad \sigma$$

$\Omega$ law

$$\sigma = \frac{e^2 n}{M\gamma}$$ Drude formula

Mobility

$$\mu = \frac{\langle v \rangle}{E} = \frac{eE}{M\gamma E} = \frac{e}{M\gamma}$$

usually introducing the scattering time

$\tau$ time laps btw 2 collisions

$$\tau = \frac{1}{\gamma}$$

## Free particle

$$\dot{p} = -\gamma p + \xi(t) + F$$ (random; Ornstein Uhlenbeck)

$$p(t) = e^{-\gamma t} p(0) + \int_0^t dt' e^{-\gamma(t-t')} (\xi(t') + F)$$

$$\dot{p} = \underbrace{-\gamma e^{-\gamma t} p(0)}_{-\gamma p} + \xi(t) \underbrace{- \gamma \int_0^t dt' e^{-\gamma(t-t')} \xi(t')}_{-\gamma p}$$

$\xi$ is random $\Rightarrow$ $p(t)$ is random

$p(t)$ is random time-dependant quantity a PROCESS or STOCHASTIC PROCESS

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

$$\langle \xi(t)\xi(t') \rangle = \frac{2M\gamma}{\beta}\delta(t-t')$$

$\xi$ is gaussian $\Rightarrow$ $p$ is gaussian

Correlation function of momenta

$$\langle p(t)\,p(t') \rangle =$$

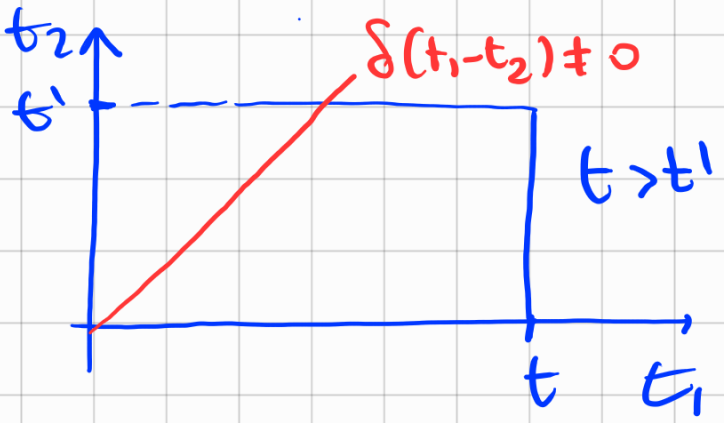
$$= e^{-\gamma(t+t')} p^2(0) +$$

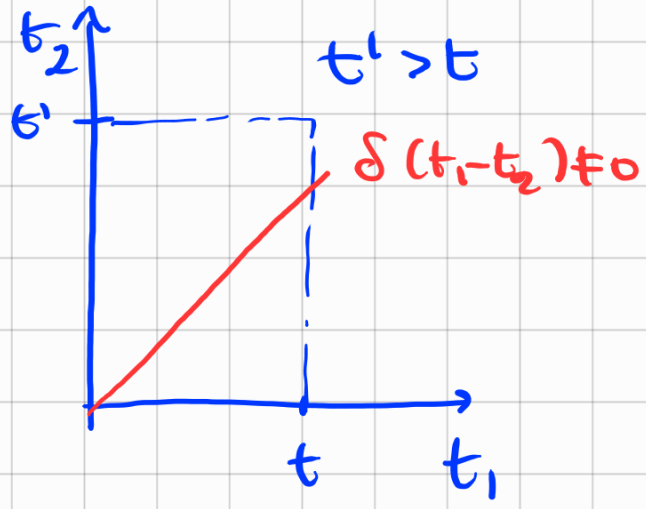
$$e^{\gamma t}\int_0^{t'} dt_2\, e^{-\gamma(t'-t_2)}\langle \xi(t_2)\rangle$$

$$e^{-\gamma t'}\int_0^{t} dt_1\, e^{\gamma(t-t_1)}\langle \xi(t_1)\rangle$$

$$+\int_0^t dt_1 \int_0^{t'} dt_2\, e^{-\gamma(t+t'-t_1-t_2)}\langle \xi(t_1)\xi(t_2)\rangle$$

$$\frac{2M\gamma}{\beta}\int_0^t dt_1 \int_0^{t'} dt_2\, e^{-\gamma(t+t'-t_1-t_2)}\,\delta(t_1-t_2)$$




$$\frac{2M\gamma}{\beta}\int_0^{\mathrm{MIN}(t,t')} dt''\, e^{-\gamma(t+t'-2t'')}$$

$\langle p(t)\,p(t')\rangle$

$$C(t,t') = e^{-\gamma(t+t')}\,p(0)^2 + \frac{M}{\beta}\left[e^{-\gamma|t-t'|} - e^{-\gamma(t+t')}\right]$$

$t=t'$

$$\langle p^2(t)\rangle = e^{-2\gamma t}\,p(0)^2 + \frac{M}{\beta}\left[1-e^{-2\gamma t}\right]$$

$(2\gamma)^{-1}$ time scale to loose memory of initial condition

$2\gamma t \gg 1 \quad \langle p^2\rangle = M/\beta$ Maxwell result

$$f(p) \propto e^{-\beta \frac{p^2}{2M}} \qquad \sigma_p^2 = \frac{M}{\beta}$$

$\langle p(t)\, p(t') \rangle \qquad t > t' \qquad t = t' + \tau \qquad \tau > 0$

$\langle p(t'+\tau)\, p(t') \rangle = C(\tau, t')$

$\gamma t' \gg 1 \qquad \tau$ finite

$$C(t,t') = e^{-\gamma(t+t')} p(0)^2 +$$

$$+ \frac{M}{\beta} \left[ e^{-\gamma |t-t'|} - e^{-\gamma(t+t')} \right]$$

$$C(\tau) = \frac{M}{\beta} e^{-\gamma \tau} \qquad (\tau > 0)$$

$\tau$: time difference — Stationary Process

$\gamma^{-1}$ time scale of decorrelation of momenta

$$\langle p(t'+\tau)\, p(t') \rangle \xrightarrow{\gamma\tau \gg 1} \langle p(t'+\tau) \rangle \langle p(t') \rangle$$

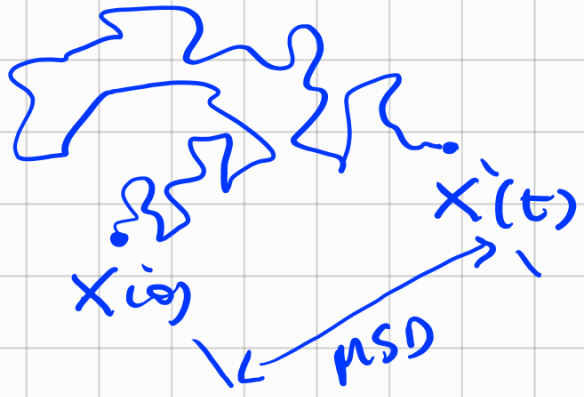
$t'+\tau$: large; $t'$: large

$\langle p(t'+\tau) \rangle \to 0 \qquad \langle p(t') \rangle \to 0$

# Diffusion of the particle

## Mean Square Displacement

$$\langle |X(t) - X(0)|^2 \rangle = \text{MSD}$$




$p(t)$ is known

$$X(t) \leftarrow \quad p(t) = M\dot{X}(t)$$

$$X(t) = \frac{1}{M}\int_0^t dt'\, p(t') + X(0)$$

$$\langle |X(t) - X(0)|^2 \rangle = \frac{1}{M}\int_0^t dt_1 \int_0^t dt_2 \underbrace{\langle p(t_1)\, p(t_2) \rangle}_{C(t_1, t_2)}$$

Exercise

# Approximate calculation in the overdamped limit for the O.U. process

$$p(t) = e^{-\gamma t} p(0) + \frac{1}{\gamma}\int_0^t dt' \underbrace{e^{-\gamma(t-t')}}_{\delta(t-t')\ \text{formal}\ \gamma\to\infty} \xi(t')$$

$$p(t) \simeq \frac{1}{\gamma}\xi(t)$$

$$x(t) = x(0) + \frac{1}{\gamma M}\underbrace{\int_0^t dt'\,\xi(t')}_{W(t)\ \text{Wiener Process}}$$

$$\langle |x(t)-x(0)|^2 \rangle = \frac{1}{\gamma^2 M^2}\int_0^t dt' \int_0^t dt'' \underbrace{\langle \xi(t')\xi(t'')\rangle}_{\frac{2M\gamma}{\beta}\delta(t'-t'')}$$

$$\langle |x(t)-x(0)|^2 \rangle = \frac{1}{\gamma^2 M^2}\frac{2M\gamma}{\beta} t$$

$$D = \frac{K_B T}{M\gamma}$$

# Diffusion

$$\langle |X(t) - X(0)|^2 \rangle = 2Dt$$

## Drift

$$\mu = \frac{e}{M\gamma} = \frac{eD}{k_B T}$$

Einstein's Relation

$\mu$ ← Dissipation

$D$ ← fluctuation