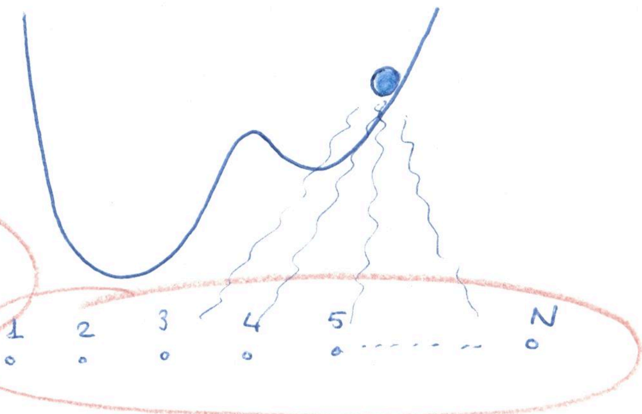
A particle interacting with N harmonic oscillators (thermal bath)

Eqs of motion & formal solution

$$H = H_S + H_B + H_{SB}$$

$$H_S = \frac{P^2}{2M} + V(X)$$



$$H_B = \sum_i \frac{p_i^2}{2m_i} + \frac{1}{2} m_i \omega_i^2 x_i^2$$

$$H_{SB} = -X \sum_i c_i x_i$$

linear coupling $\Rightarrow$ formal solution

Hamilton's equation

$$\begin{cases} \dot{X} = \frac{\partial H}{\partial P} = \frac{P}{M} \\ \dot{P} = -\frac{\partial H}{\partial X} = -\frac{\partial V}{\partial X} + \sum_i c_i x_i \end{cases}$$

forcing terms

$$\begin{cases} \dot{x}_i = \frac{\partial H}{\partial p_i} = \frac{p_i}{m_i} \\ \dot{p}_i = -\frac{\partial H}{\partial x_i} = -m_i \omega_i^2 x_i + c_i X \end{cases}$$

$\Rightarrow$ driven harmonic oscillators

Solve formally the harmonic part 2

$$X_i(t) = X_i^{(0)}(t) + \frac{c_i}{m_i\omega_i}\int_0^t dt' \sin\omega_i(t-t')X(t')$$

$$P_i(t) = P_i^{(0)}(t) + c_i\int_0^t dt' \cos\omega_i(t-t')X(t')$$

in absence of driving force

particular solution

$$X_i^{(0)}(t) = x_i(0)\cos\omega_i t + \frac{P_i(0)}{m_i\omega_i}\sin\omega_i t$$

$$P_i^{(0)}(t) = p_i(0)\cos\omega_i t - m_i x_i(0)\sin\omega_i t$$

here w_i is missing

proof:

$$\dot{P}_i(t) = \underbrace{\dot{P}_i^{(0)}}_{-m_i\omega_i^2 X_i^{(0)}(t)} + c_i X(t) - \underbrace{c_i\int_0^t dt' \sin\omega_i(t-t')X(t')}_{-m_i\omega_i^2[X_i(t) - X_i^{(0)}(t)]}$$

$$= -m_i\omega_i^2 X_i(t) + c_i X(t)$$

the same for $\dot{X}_i$

substitute the formal solution for $X_i(t)$ into the equation for $\dot{X}$ and get a closed equation for $\dot{X}$

$$M\ddot{X} = -\frac{\partial V}{\partial X} + \Sigma_i c_i \left(x_i^{(0)} + \frac{c_i}{m_i \omega_i} \int_0^t dt' \sin\omega_i(t-t') X(t') \right)$$

make a trick in the integral to make $\dot{X}$ appear

$$\int_0^t dt' \sin\omega_i(t-t') X(t') = \frac{1}{\omega_i} \int dt' \left(\frac{\partial}{\partial t'} \cos\omega_i(t-t') \right) X(t')$$

by parts

$$= \frac{1}{\omega_i^2} [\cancel{\cos\omega_i t} \, X(t) - \cos\omega_i t \, X(0)] - \frac{1}{\omega_i} \int_0^t dt' \cos\omega_i(t-t') \dot{X}(t')$$

$$M\ddot{X} = -\frac{\partial V}{\partial X} + \Sigma_i c_i x_i^{(0)}(t) + \left(\Sigma_i \frac{c_i^2}{m_i \omega_i^2} \right) X(t) - \left(\Sigma_i \frac{c_i^2}{m_i \omega_i^2} \cos\omega_i(t) \right) X(0)$$

$$- \Sigma_i \frac{c_i^2}{m_i \omega_i^2} \int_0^t dt' \cos\omega_i(t-t') \dot{X}(t')$$

define the Memory-Friction Kernel

$$\boxed{\gamma(t-t') = \Theta(t-t') \frac{1}{M} \Sigma_i \frac{c_i^2}{m_i \omega_i^2} \cos\omega_i(t-t')}$$

re-define x

$$\gamma(0^+) = \frac{1}{M} \Sigma_i \frac{c_i^2}{m_i \omega_i^2}$$

$$M\ddot{X} = -\frac{\partial V}{\partial X} + \Sigma_i c_i x_i^{(0)}(t) + M\gamma(0^+) X(t) - M\gamma(t) X(0) -$$

$$- \int_{-\infty}^t dt' \gamma(t-t') \dot{X}(t')$$

re-define V

shift x_i and re-define V
in order to get a:

a) external zero mean noise term

b) friction (memory) term

c) potential term

in the equation for $\ddot{X}$

the presence of the particle modify the equilibrium position of the oscillators

Consider

$$H' = H_B + H_{SB} = \Sigma_i \frac{p_i^2}{2m_i} + \frac{1}{2} m_i \omega_i^2 x_i^2 - c_i x_i X$$

$$\frac{\partial H'}{\partial x_i} = m_i \omega_i^2 x_i - c_i X$$

equilibrium position $\quad x_i^{eq} = \frac{c_i}{m_i \omega_i^2} X$

1) shift the initial position
and leave p_is unchanged

$$y_i(0) = x_i(0) - x_i^{eq}(0)$$

$$\Sigma_i c_i x_i^{(0)}(t) - M\gamma(t) X(0) = \Sigma_i c_i y_i^{(0)}(t)$$

$$\Sigma_i c_i y_i^{(0)}(t) = \Sigma_i c_i x_i^{(0)}(t) - \Sigma_i \frac{c_i^2}{m_i \omega_i^2} X(0) \cos \omega_i t$$

2) Re-define V

$$\tilde{V}(X) = V(X) - \frac{1}{2} M \gamma(0) X^2$$

such as

$$\frac{\partial \tilde{V}}{\partial X} = \frac{\partial V}{\partial X} - M\gamma(0) X$$

Potential

Noise

Friction

then

$$M\ddot{X} = -\frac{\partial \tilde{V}}{\partial X} + \underbrace{\sum_i c_i y_i^{(0)}(t)}_{\xi_i(t)} - M\int_{-\infty}^{t} dt' \gamma(t-t') \dot{X}(t)$$

where

$$y_i^{(0)}(t) = \cos\omega_i t \; y_i(0) + \sin\omega_i t \; \frac{p_i(0)}{m_i \omega_i}$$

$$p_i^{(0)}(t) = \cos\omega_i t \; p_i(0) - \sin\omega_i t \; m_i y_i(0)$$

here w_i is missing

this is formal and still valid for any # of oscillators

Now

$N \to \infty$ at any given time t

this is accomplished into 2 steps

1) introduce statistics of initial data 2) $N \to \infty$

properties of the noise term:
the action of the thermal bath
"Average" over initial data

$\Rightarrow \{ y_i(0), p_i(0) \}$ from Boltzmann's thermal distribution

$y_i(0), p_i(0)$ are zero mean independent gaussian variables

Bath Temp

$$P(y_i) \propto e^{-\beta \frac{1}{2} m_i \omega_i^2 y_i^2} \longrightarrow \langle y_i^2 \rangle = \frac{1}{\beta m_i \omega_i^2}$$

$$\beta = \frac{1}{k_B T}$$

$$P(p_i) \propto e^{-\beta \frac{p_i^2}{2 m_i}} \longrightarrow \langle p_i^2 \rangle = \frac{m_i}{\beta}$$

consider an ensemble of initial data and average on it

$$\xi_i(t) = \sum_i c_i \, y_i^{(0)}(t)$$

is a sum of gaussian variables $\Rightarrow$ is a gaussian variable

with zero mean

average over initial data

$$\langle \xi(t) \rangle = \sum_i c_i \langle y_i^{(0)}(t) \rangle =$$

$$= \sum_i c_i \cos \omega_i t \underbrace{\langle y_i(0) \rangle}_{0} + \frac{c_i}{m_i \omega_i} \sin \omega_i t \underbrace{\langle p_i(0) \rangle}_{0} = 0$$

and correlation function

$$\langle \xi_i(t)\, \xi_i(t') \rangle = \sum_{ij} c_i c_j \langle y_i^{(0)}(t)\, y_j^{(0)}(t') \rangle$$

$$\langle y_i^{(0)}(t)\, y_j^{(0)}(t') \rangle = \delta_{ij} \langle y_i^{(0)}(t)\, y_i^{(0)}(t') \rangle$$

because each $y_i(0)$, $p_i(0)$ are statistically independent $\Rightarrow$ initially each oscillator has an independent velocity/position

$$\langle y_i^{(0)}(t)\, y_i^{(0)}(t') \rangle = \langle y_i^2(0) \rangle \cos\omega_i t \cos\omega_i t' +$$

$$+ \frac{1}{m_i^2 \omega_i^2} \langle p_i^2(0) \rangle \sin\omega_i t \sin\omega_i t' +$$

$$+ \frac{1}{m_i \omega_i} \cancel{\langle x_i(0)\, p_i(0) \rangle} (\cos\omega_i t \sin\omega_i t' + \sin\omega_i t \cos\omega_i t')$$

position & velocity are independent

$$= \frac{1}{\beta m_i \omega_i^2} (\cos\omega_i t \cos\omega_i t' + \sin\omega_i t \sin\omega_i t')$$

$$= \frac{1}{\beta m_i \omega_i^2} \cos\omega_i (t - t')$$

$$\boxed{\langle \xi_i(t)\, \xi_i(t') \rangle = \frac{M}{\beta} \gamma(t-t') \quad t>t'}$$

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

$$\langle \xi(t) \rangle = 0 \qquad \langle \xi(t)\,\xi(t') \rangle = \frac{M}{\beta}\,\gamma(t-t')$$

$$\beta = \frac{1}{k_B T}$$

statistical properties of the NOISE ξ_e

Memory-Friction Kernel

friction & memory

for a small number of oscillators

$$\gamma(t-t') = \Theta(t-t')\,\frac{1}{M}\sum_{i=1}^{N} \frac{c_i^2}{m_i \omega_i^2} \cos\omega_i (t-t')$$

is a sum of a small # of oscillating functions $\Rightarrow$ is ~~quasi~~ periodic

we do not have a real friction

we need $N \to \infty$

The $N \to \infty$ limit

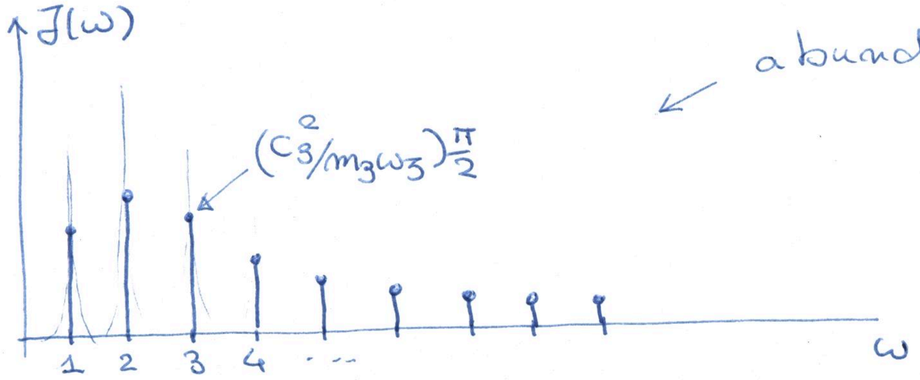
Ohmic spectral density

introduce the spectral density

$$\boxed{J(\omega) = \frac{\pi}{2} \sum_i^N \frac{c_i^2}{m_i \omega_i} \delta(\omega - \omega_i)}$$

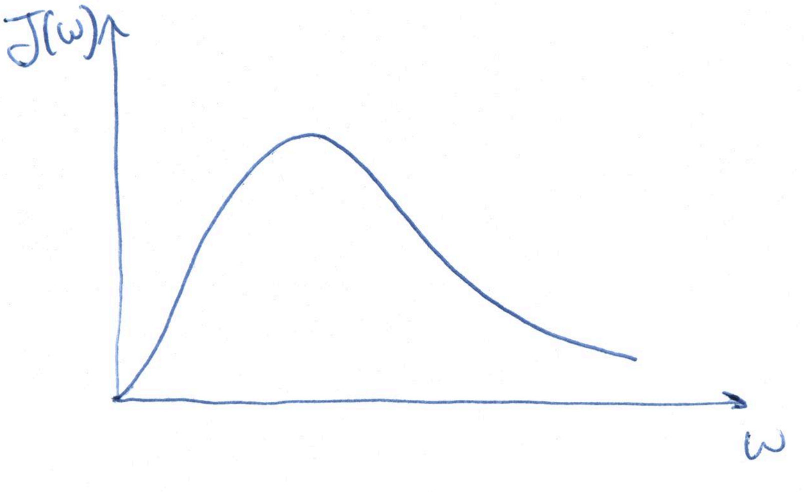
suppose that we choose all $m_i = 1$ and equispaced ω_i

$\omega_i = i \Delta\omega \quad i = 1, N$



a bunch of δ function

as $N \to \infty$ we may imagine that the bunch of δ functions collapses into a continuum distribution



the memory-friction kernel can be expressed formally in terms of $J(\omega)$

$$\sum_{i=1}^{N} \frac{c_i^2}{m_i\omega_i^2}\cos\omega_i(t-t') = \frac{2}{\pi}\int_0^\infty d\omega\, \frac{J(\omega)}{\omega}\cos[\omega(t-t')]$$

proof by subst the def of J into

$$\frac{\cancel{2}}{\cancel{\pi}}\int_0^\infty d\omega\, \frac{1}{\omega}\, \frac{\cancel{\pi}}{\cancel{2}}\sum_{i=1}^{N} \frac{c_i^2}{m_i\omega_i}\,\delta(\omega-\omega_i)\,\cos[\omega(t-t')] =$$

since all $\omega_i > 0$!

$$= \sum_{i=1}^{N} \frac{c_i^2}{m_i\omega_i^2}\cos[\omega_i(t-t')]$$

$$\boxed{\gamma(t-t') = \Theta(t-t')\,\frac{2}{\pi M}\int_0^\infty d\omega\, \frac{J(\omega)}{\omega}\cos[\omega(t-t')]}$$

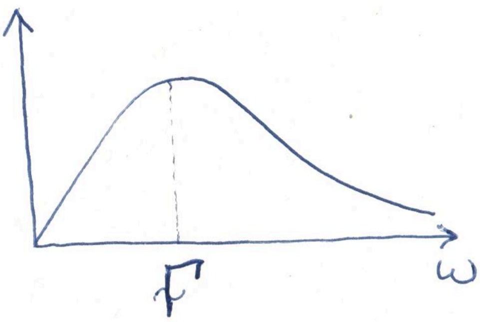
Memory Friction Kernel

Spectral Density

$\boxed{N\to\infty}$ $J(\omega)$ smooth function

Ohmic Spectral Density

$$\boxed{J(\omega) = M\gamma\,\frac{\omega\,\Gamma^2}{\omega^2+\Gamma^2}}$$



Calculation of Memory-Friction using Ohmic spectral density

$$\gamma(t-t') = \Theta(t-t') \frac{2}{\cancel{M}\pi} \int_0^\infty d\omega \, \frac{1}{\cancel{\omega}} \, M\gamma \, \frac{\cancel{\omega}\Gamma^2}{\omega^2+\Gamma^2} \cos\omega(t-t')$$

$$= \Theta(t-t')\, \gamma \, \underbrace{\frac{2}{\pi} \int_0^\infty d\omega \, \frac{\Gamma^2}{\omega^2+\Gamma^2} \cos\omega(t-t')}_{\Gamma e^{-\Gamma|t-t'|}}$$

$$\boxed{\gamma(t-t') = \Theta(t-t')\, \gamma \, \Gamma e^{-\Gamma|t-t'|}}$$

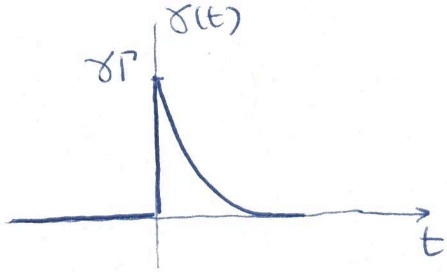
decay rate of memory kernel

$$\boxed{\langle \xi_e(t)\, \xi_e(t') \rangle = \frac{M\gamma}{\beta} \Gamma e^{-\Gamma|t-t'|}}$$

decay rate of noise correlations

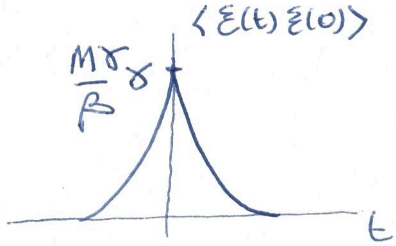
White noise limit
Langevin equation

An affordable equation for $X(t)$ is obtained in the limit $\boxed{\Gamma \to \infty}$



$$\boxed{\gamma(t-t') \longrightarrow \gamma\,\delta(t-t')}$$

$$\int_{-\infty}^{+\infty} dt\, \gamma(t) = \int_0^{\infty} dt\, \gamma\Gamma e^{-\Gamma t} = \gamma \cancel{\Gamma} \frac{1}{\cancel{\Gamma}}$$



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

$$\int_{-\infty}^{+\infty} dt \langle \xi(t)\,\xi(0)\rangle = \frac{M\gamma}{\beta}\,\Gamma \int_{-\infty}^{+\infty} dt\, e^{-\Gamma|t|} = \frac{M\gamma}{\beta}\cancel{\Gamma}\frac{2}{\cancel{\Gamma}}$$

Langevin equation

$$M\ddot{X} = -\frac{\partial \tilde{V}}{\partial X} + \xi(t) - M\gamma\,\dot{X}(t)$$

$$\boxed{\dot{p} = -\frac{\partial \tilde{V}}{\partial X} + \xi(t) - \gamma p}$$

White noise

friction