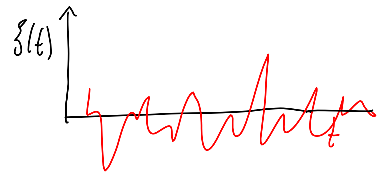
HO oscillator with classical noise

HON1

$$m\ddot{x} + m\gamma\dot{x} + m\Omega^2 x = \xi(t) \qquad (1)$$

"Langevin equation"

noisy force



noise average $\langle \xi(t) \rangle = 0$ (2)

Noise correlator: $\langle \xi(t)\xi(0)\rangle = \eta\,\delta(t)$ (3)

η constant has to be adjusted such that $\frac{1}{2}M\Omega^2\langle x^2\rangle = \frac{1}{2}k_BT$

Fourier transform:

$$\tilde{x}_\tau[\omega] = \frac{1}{\sqrt{\tau}}\int_0^\tau dt\, e^{i\omega t}\, x(t) \qquad (4a)$$

(subscript τ will be dropped below)

$$\tilde{\xi}_\tau[\omega] = \frac{1}{\sqrt{\tau}}\int_0^\tau dt\, e^{i\omega t}\, \xi(t) \qquad (4b)$$

HON2

Now: $\langle |\xi[\omega]|^2 \rangle = \langle \tilde{\xi}[\omega]\,\tilde{\xi}[-\omega]\rangle$ (1)

$$= \frac{1}{\tau}\int_0^\tau dt \int_0^\tau dt'\, e^{i\omega(t-t')}\, \underbrace{\langle \xi(t)\xi(t')\rangle}_{\overset{(1.3)}{=}\ \eta\,\delta(t-t')} \qquad (2)$$

$$= \frac{1}{\tau}\int_0^\tau dt\, \eta = \eta \qquad (3)$$

$\Longrightarrow$ Noise spectrum is frequency-independent: "white noise".

How does it affect the power spectrum $S_{xx}[\omega] = \langle |x[\omega]|^2\rangle$?

$\boxed{\text{HON3}}$

$$\frac{m}{\sqrt{\tau}}\int_0^\tau dt\, e^{i\omega t}\left[\ddot{x} + \gamma\dot{x} + \Omega^2 x\right] = \frac{1}{\sqrt{\tau}}\int_0^\tau dt\, e^{i\omega t}\,\xi(t) \qquad (1)$$

integrate by parts, boundary terms vanish in limit $\tau \to \infty$:

$$\frac{1}{\sqrt{\tau}}\int_0^\tau dt\, e^{i\omega t}\frac{dx}{dt} = \frac{1}{\sqrt{\tau}}\int_0^\tau dt \left(\underbrace{-\frac{d}{dt}}_{-i\omega} e^{i\omega t}\right) x + \frac{1}{\sqrt{\tau}}\Big[e^{i\omega t} x\Big]_0^\tau$$

$\simeq 0$ for $\tau \to \infty$

$$x(t) \to \tilde{x}[\omega], \qquad \dot{x}(t) \to -i\omega\,\tilde{x}[\omega], \qquad \ddot{x}(t) \to -\omega^2\,\tilde{x}[\omega]$$

$$m\left[-\omega^2 - i\gamma\omega + \Omega^2\right]\tilde{x}[\omega] = \tilde{\xi}[\omega]$$

$$\tilde{x}[\omega] = \underbrace{\frac{1}{m\left(-\omega^2 - i\gamma\omega + \Omega^2\right)}}_{\equiv A(\omega)}\,\tilde{\xi}[\omega]$$

A is a "dynamic susceptibility." It specifies how strongly system reacts to driving at frequency ω.

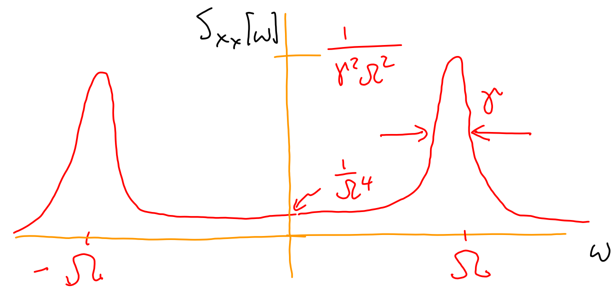
$\boxed{\text{HON4}}$

$$\Rightarrow \qquad \tilde{x}^*[\omega] = \underbrace{A^*(\omega)}_{A(-\omega)}\,\tilde{\xi}^*[\omega] \qquad (1)$$

then

$$S_{xx}[\omega] = \langle|\tilde{x}[\omega]|^2\rangle = |A(\omega)|^2\,\langle|\tilde{\xi}[\omega]|^2\rangle \qquad (2)$$

$$= \frac{\eta/m^2}{(\Omega^2-\omega^2)^2 + \gamma^2\omega^2} \qquad (3)$$



for $\Omega \gg \gamma$ we can approximate peaks by Lorenzians:

$$S_{xx}(\omega) \simeq \eta/m^2 \left[\underbrace{\frac{\frac{1}{\pi}\,\gamma/2}{(\omega+\Omega)^2 + (\gamma/2)^2}}_{\delta_\gamma(\omega+\Omega)} + \underbrace{\frac{\frac{1}{\pi}\,\gamma/2}{(\omega-\Omega)^2 + (\gamma/2)^2}}_{\delta_\gamma(\omega-\Omega)}\right]\frac{1}{4\Omega^2}\,\frac{2\pi}{\gamma} \qquad (4)$$

= broadened δ-fnct.

$$\simeq \frac{\pi\eta}{2m^2\Omega^2\gamma}\left[\delta_\gamma(\omega+\Omega) + \delta_\gamma(\omega-\Omega)\right] \qquad (5)$$

Check replacement by Lorenzians for $\Omega \gg \gamma$:

HOW5

$$\frac{m^2}{\eta} S_{xx}(\omega) = \frac{1}{(\Omega^2-\omega^2)^2 + \gamma^2\omega^2} \overset{\Omega \gg \gamma}{\simeq} \frac{1}{(\Omega^2-\omega^2)^2 + \gamma^2\Omega^2}$$

$$\frac{m^2}{\eta} S_{xx}(\Omega) = \frac{1}{\gamma^2\Omega^2}$$

FWHM? $\quad \frac{1}{2} = \frac{A(\Omega)}{A(\Omega \pm \delta/2)} = \frac{\gamma^2\Omega^2}{(\Omega^2 - (\Omega \pm \delta/2)^2)^2 + \gamma^2\Omega^2}$

$$\Rightarrow \quad = \frac{\gamma^2\Omega^2}{(\mp\Omega\delta - \cancel{\delta^2/4})^2 + \gamma^2\Omega^2} \quad \Rightarrow \quad \delta = \gamma = \text{FWHM}$$

Approximate peaks by Lorenzians with FWHM $= \gamma$, height $= \frac{1}{\gamma^2\Omega^2}$:

$$\frac{m^2}{\eta} S_{xx}(\omega) \simeq \left[\frac{1}{(\omega-\Omega)^2 + (\gamma/2)^2} + \frac{1}{(\omega+\Omega)^2 + (\gamma/2)^2}\right] \frac{1}{4\Omega^2}$$

HOW6

Weight? use $\quad \int d\omega\, \delta_\gamma(\omega) = \int_{-\infty}^{\infty} dx \frac{\gamma/\pi}{{}^2 + \gamma^2} = 1 \qquad (1)$

$$\Rightarrow \langle x^2\rangle = \int \frac{d\omega}{2\pi} S_{xx}(\omega) = \frac{\cancel{\pi}\,\eta}{2m^2\Omega^2\gamma}\,\cancel{2}\cdot\frac{1}{\cancel{2\pi}} \qquad (2)$$

To get equipartition, $\langle x^2\rangle \overset{!}{=} \frac{k_B T}{M\Omega^2}$, we must choose $\qquad (3)$

$$\Rightarrow \frac{\eta}{m^2}\frac{1}{\Omega^2}\frac{1}{2\gamma} = \frac{k_B T}{m\Omega^2} \Rightarrow \boxed{\eta = 2\gamma m k_B T} \qquad (4)$$

$\Rightarrow$ to get equilibrium behavior at temperature T, strength of stochastic force must be proportional to strength of dissipation!

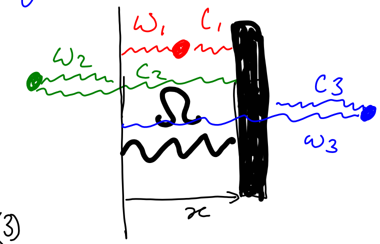
(which makes sense!)

HO oscillator with quantum noise : Caldeira-Leggett-Model

$\boxed{\text{HOW7}}$

$$H = H_S + H_B \qquad (1)$$

"particle x is coupled by springs to harmonic oscillators"



$$H_S = \frac{p^2}{2m} + \frac{1}{2} m \Omega^2 x^2 \qquad (2)$$

$$H_B = \sum_{i=1}^{N} \left(\frac{p_i^2}{2m_i} + \frac{1}{2} m_i \omega_i^2 q_i^2 \right) \qquad (N \to \infty) \qquad (3)$$

$$H_{SB} = \underbrace{- q \sum_{i=1}^{N} c_i q_i}_{} + \underbrace{x^2 \sum_{i=1}^{N} \frac{c_i^2}{2 m_i \omega_i^2}}_{= \text{counterterm}} \qquad (4)$$

$$\text{"Force"} = \frac{\partial H_{SB}}{\partial x} = - \sum_{i=1}^{N} c_i q_i \qquad (5)$$

is sum of stochastic variables.

$[c_i]$ has units of $[m_i \omega_i^2]$

Effective potential for bath oscillators:

$$\frac{1}{2} m_i \omega_i^2 \Big(\underbrace{q_i - \frac{x c_i}{m_i \omega_i^2}}_{\delta q_i \text{ has "free oscillations"}} \Big)^2 \qquad (6)$$

$\boxed{\text{HOW8}}$

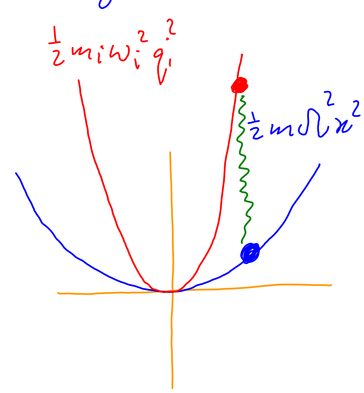
Why is counterterm needed? To ensure that x feels effective potential $\frac{1}{2} m \Omega^2 x^2$, plus noise (but not the harmonic potential of bath oscillators)

For given x, all the oscillators shift to minimize their potential,

$$V_i(q_i) = \frac{1}{2} m_i \omega_i^2 q_i^2 - x c_i q_i$$

$$0 = \frac{\partial V_i}{\partial q_i} \quad \Rightarrow \quad q_i^{min} = \left(\frac{c_i}{m_i \omega_i^2} \right) x$$

$$\sum_i V_i(q_i^{min}) = - \frac{1}{2} \sum_i \frac{c_i^2}{m_i \omega_i^2} x^2$$



this is x-dependent, hence this would modify the potential felt by x.

The counterterm in (7.4) is chosen such that it cancels this contribution.

Equations of motion:

HOW9

Heisenberg: $$\frac{d\tilde{A}}{dt} = -\frac{i}{\hbar}[\hat{A},\hat{H}] \quad (1)$$

$$H = \frac{p^2}{2m} + \frac{1}{2} m \Omega^2 x^2 + \sum_{i=1}^{N} \left[\frac{p_i^2}{2m_i} + \frac{1}{2} m_i \omega_i^2 q_i^2 - x c_i q_i + x^2 \frac{c_i^2}{2 m_i \omega_i^2} \right] \quad (2)$$

$$\hat{A} = x: \quad \dot{x} = \frac{-i}{\hbar}[x, H] = \frac{-i}{\hbar}\frac{1}{2m} 2 \overbrace{i\hbar}^{[x,p]} p = \frac{p}{m} \quad (3)$$

$$\ddot{x} = \frac{1}{m}\dot{p} = -\frac{i}{\hbar}[p, H] = -x\left[\Omega^2 + \frac{1}{m}\sum_i \frac{c_i^2}{m_i \omega_i^2}\right] + \underbrace{\frac{1}{m}\sum_i c_i q_i}_{\xi(t)} \quad (4)$$

$$\Rightarrow \boxed{m\ddot{x}(t) + \left(m\Omega^2 + \sum_i \frac{c_i^2}{m_i \omega_i^2}\right)x = \sum_i c_i q_i(t)} \quad (5)$$

the bath provides a fluctuating force!

to find its dynamics, we need eq. of motion for q_i!

Completely analogous: $(x \leftrightarrow q_i,\ p \leftrightarrow p_i,\ m \leftrightarrow m_i)$ (no counterterm)

HON10

$$\boxed{\ddot{q}_i(t) + \omega_i^2 q_i(t) = \frac{c_i}{m_i} x(t)} \quad (1)$$

$x(t)$ acts like driving force for bath oscillator.

Solution of (1), for given "driving" $x(t)$: $$q_i(t) = q_i^{(h)}(t) + q_i^{(p)} \quad (2)$$

$$q_i^{(h)}(t) = \left[q_i(0) \cos\omega_i t + \dot{q}_i(0)\frac{1}{\omega_i}\sin\omega_i t \right] \quad (3)$$

(a) (b)

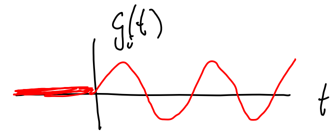
solution homogeneous eq., with proper boundary cond.

$$q_i^{(p)}(t) = \frac{c_i}{m_i}\int_0^\infty dt'\, G_i(t-t')\, x(t') \quad (4)$$

particular solution to inhom. eq.

where Green's function satisfies: $$(\partial_t^2 + \omega_i^2) G_i(t-t') = \delta(t-t') \quad (5)$$

and is given by $$G_i(t) = \theta(t) \frac{\sin\omega_i t}{\omega_i} \quad (6)$$



Check: (10.6) $\quad \partial_t G_i(t) = \frac{1}{\cancel{\omega_i}}\Big[\,\underbrace{\delta(t)\sin\omega_i t}_{=0 \text{ at } t=0} + \cancel{\omega_i}\,\theta(t)\cos\omega_i t\Big]$ HON 11

$$\partial_t^2 G_i(t) = \delta(t)\underbrace{\cos\omega_i t}_{=1 \text{ at } t=0} - \theta(t)\,\omega_i \sin\omega_i t$$

$$= \delta(t) - \omega_i^2 G_i(t) \quad \checkmark \quad \text{agrees with (10.5)}$$

For later convenience:

$$q_i^{(p)} = \frac{c_i}{m_i}\int_0^{\cancel{\infty}\, t} dt'\, \cancel{\theta(t-t')}\,\frac{\sin\omega_i(t-t')}{\omega_i}\,x(t')$$

integrate by parts: $\quad = \frac{c_i}{m_i\omega_i^2}\left[-\int_0^t dt' \cos\omega_i(t-t')\,\dot{x}(t') + \left[x(t) - x(0)\cos\omega_i t\right]\right]$ (c) (d) (e)

$$\sin\omega(t-t')\,x = \frac{d}{dt'}\left\{\frac{\cos\omega(t-t')}{\omega}\,x\right\} - \frac{\cos\omega(t-t')}{\omega}\,\frac{dx}{dt'}$$

"Eliminate" q_i's by inserting (10.2) into (9.5): HON12

(9.5)

$$\underset{①}{m\ddot{x}(t)} + \Big(\underset{②}{m\Omega^2} + \underset{③}{\sum_i \frac{c_i^2}{m_i\omega_i^2}}\Big)x(t) = \sum_i c_i\Big[\underset{④}{q_i^{(h)}(t)} + \underset{⑤}{q_i^{(p)}(t)}\Big] \tag{1}$$

$$= \sum_i c_i\Big[\underset{4a}{q_i(0)\cos\omega_i t} + \underset{4b}{\dot{q}_i(0)\,\frac{1}{\omega_i}}\sin\omega_i t\Big] \tag{2}$$

cancel!

$$- m\int_0^t dt'\,\underbrace{\frac{1}{m}\sum_i \frac{c_i^2}{m_i\omega_i^2}\cos\omega_i(t-t')}_{=\gamma(t-t')}\,\underset{5c}{\dot{x}(t')} \quad \sum_i \frac{c_i^2}{m_i\omega_i^2}\Big[\underset{5d}{x(t)} - \underset{5e}{x(0)\cos\omega_i t}\Big] \tag{3}$$

$$\boxed{\underset{①}{m\ddot{x}} + \underset{②}{m\Omega^2 x} + \underset{5c}{m\int_0^t dt'\,\gamma(t-t')\,\dot{x}(t')} = \xi(t)} \quad \text{effective fluctuating force} \tag{4}$$

damping term ["retarded" in time: value at t depends on all $x(t')$ for $t' < t$.]

$$\xi(t) \equiv \sum_i c_i\Big\{\Big[\underbrace{\underset{4a}{q_i(0)} - \underset{5e}{\frac{c_i}{m_i\omega_i^2}x(0)}}_{\delta q_i(0) \quad \text{see (7.6)}}\Big]\cos\omega_i t + \underset{4b}{\frac{P_i(0)}{m_i\omega_i}}\sin\omega_i t\Big\} \tag{5}$$

$\boxed{\text{HON13}}$

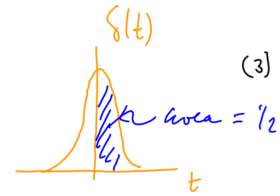
Note: $\langle \xi(t) \rangle = 0$, since $\langle \delta q_i(0) \rangle = 0$, $\langle p_i(0) \rangle = 0$ $\Big\}$ initial values are random

Damping function:

$$\gamma(t) = \frac{1}{m}\, 2 \int_0^\infty \frac{d\omega}{\pi} \underbrace{\pi \sum_i \frac{c_i^2}{2 m_i \omega_i}\, \delta(\omega-\omega_i)}_{\equiv\, J(\omega)\ \text{spectral function for bath-system coupling!}} \frac{\cos \omega_{\cancel{i}} t}{\omega_{\cancel{i}}} = \frac{2}{m} \int_0^\infty \frac{d\omega}{\pi}\, J(\omega) \cos \omega t \qquad (1)$$

Assume "ohmic" bath: $J(\omega) \equiv m\gamma\omega$ (2)

$$\Rightarrow \quad \gamma(t) = \gamma \int_0^\infty \frac{d\omega}{\pi} \left(e^{i\omega t} + e^{-i\omega t} \right) = 2\gamma\, \delta(t) \qquad (3)$$



Damping term in (12.4):

$$m \int_0^t dt'\, \gamma(t-t')\, \dot{x}(t') = m\gamma 2 \int_0^t dt'\, \delta(t-t')\, \dot{x}(t') = m\gamma\dot{x}(t) \qquad (4)$$

$\Rightarrow$ $\boxed{\text{Ohmic bath gives "velocity-proportional" damping } m\gamma\dot{x}}$!!!

$\boxed{\text{HON14}}$

Bath correlation function: $\langle \xi(t)\, \xi(0) \rangle = \,?$

$$\xi(t) = \sum_i c_i \left[\delta q_i(0) \cos \omega_i t + \frac{p_i(0)}{m_i \omega_i} \sin \omega_i t \right]$$

dynamics of $\delta q_i(0)$, $p_i(0)$ is governed by $H_i \overset{(7.3,\,7.4)}{=} \frac{1}{2}\frac{p_i^2}{2m_i} + \frac{1}{2} m_i \omega_i^2 (\delta q_i^2)$

so:

$$\langle \delta q_i(0)\, \delta q_j(0) \rangle = \frac{\hbar}{2 m_i \omega_i}\, \delta_{ij} \left(2 n_B(\omega_i) + 1 \right)$$

$\boxed{\text{see NM14}}$

$$\langle p_i(0)\, \delta q_j(0) \rangle = -\frac{i\hbar}{2}\, \delta_{ij}$$

$$n(\omega_i) \equiv \frac{1}{e^{\beta\omega_i\hbar} + 1}$$

$\boxed{\text{see NM15}}$

$$\langle \xi(t)\, \xi(0) \rangle = \hbar \sum_i \frac{c_i^2}{2 m_i \omega_i} \left[n(\omega_i)\, e^{i\omega_i t} + (n(\omega_i)+1)\, e^{-i\omega_i t} \right]$$

$$S_{\xi\xi}(\omega) = \langle |\xi(\omega)|^2 \rangle = \hbar \int_0^\infty d\bar{\omega}\; 2 \underbrace{\pi \sum_i \frac{c_i^2}{2 m_i \omega_i}\, \delta(\bar{\omega} - \omega_i)}_{J(\bar{\omega}) \,=\, m\gamma\bar{\omega}} \left[n(\bar{\omega})\, \delta(\omega + \bar{\omega}) + (n(\bar{\omega})+1)\, \delta(\omega - \bar{\omega}) \right]$$

$$S_{\xi\xi}(\omega) = 2\hbar m\gamma \left[\Theta(-\omega)\,(-\omega\, n(-\omega)) + \Theta(\omega)\,(\omega\,(n(\omega)+1)) \right] \qquad \boxed{\text{HOW15}}$$

mehr Gewicht bei positiven Frequenzen!

Check: large-temperature-limit: $\hbar\omega n(\omega) = \frac{\omega}{e^{\hbar\omega/Tk_B}-1} \overset{T\gg\hbar\omega}{\simeq} \frac{k_B T}{\hbar}$

$$S_{\xi\xi}(\omega) \xrightarrow{k_BT\gg\hbar\omega} 2\, m\gamma\, k_B T = \eta \quad (\text{in notation of } 2.3)$$

↳ large-T limit reproduces (6.4) !!

What does this imply for damped particle?

$$S_{xx}[\omega] = \langle|\tilde{x}[\omega]|^2\rangle = |A(\omega)|^2\,\langle|\tilde{\xi}[\omega]|^2\rangle$$

$$\overset{\Omega\gg\gamma \text{ use } (4.3)}{\simeq} \frac{\eta/m^2}{(\Omega^2-\omega^2)^2+\gamma^2\omega^2}\, S_{\xi\xi}(\omega)$$

If we approximate $|A(\omega)|^2$ by (4.4), sum of two Lorentzians, we get $\boxed{\text{HOW16}}$

$$S_{xx}(\omega) = \frac{\pi}{\cancel{2}m^{\cancel{2}}\Omega^2\cancel{\gamma}}\left[\delta_\gamma(\omega+\Omega) + \delta_\gamma(\omega-\Omega)\right]$$

$$\times\ \cancel{2}\hbar\cancel{m\gamma}\left[\Theta(-\omega)\,(-\omega\, n(-\omega)) + \Theta(\omega)\,(\omega\,(n(\omega)+1))\right]$$

$$= \underbrace{\frac{\hbar}{2m\Omega^2}}_{\Omega\, x_{ZPF}^2}\, 2\pi\left[\delta_\gamma(\omega+\Omega)\,(-\omega\, n(-\omega)) + \delta_\gamma(\omega-\Omega)\,\omega\,(n(\omega)+1)\right]$$

for $\Omega\gg\gamma$, we can replace ω by Ω due to δ_γ-peaks:

$$\simeq 2\pi\, x_{ZPF}^2\left[\delta_\gamma(\omega+\Omega)\, n(\Omega) + \delta_\gamma(\omega-\Omega)\,(n(\Omega)+1)\right]$$

$$\langle x^2\rangle = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\, S_{xx}(\omega) = x_{ZPF}^2\cdot(2n(\Omega)+1) = \frac{\hbar}{2m\Omega}\coth\frac{\hbar\Omega}{2k_BT} \xrightarrow{k_BT\gg\hbar\Omega} \frac{k_BT}{m\Omega^2}\ ✓$$

So, in classical limit $k_BT\gg\hbar\Omega$, we recover equipartition!!