Lecture 10: Heisenberg-Langevin Equations

In the last lecture we saw how the problem of a system coupled to a bath of harmonic oscillators gave rise to Fokker-Planck equation describing the system's distribution function. This equation giving rise to drift and diffusion evolution are familiar in classical nonequilibrium statistical physics. They describe the evolution of an ensemble ~~ensemble~~ of particles, each undergoing "Brownian motion", under the influence a stochastic fluctuating force. The stochastic evolution of a single trajectory is described by a "Langevin" Eq.

As we will see shortly, the Heisenberg equations of motion for the system operators, coupled to the reservoir, take the form of Langevin equations. To understand their behavior, we first turn to classical problem.

Classical Brownian Motion (From C.T. sect. C_{IV} ·1)

Brownian motion describes the random, irregular motion of a particle suspended in a liquid, original observed by Robert Brown in 1827. Einstein, in 1905, explained the phenomenon through a "molecular" picture of the fluid. It was one of the most important results in establishing the ~~the~~ atomist picture of matter at the turn of the $19^{th} \to 20^{th}$ century

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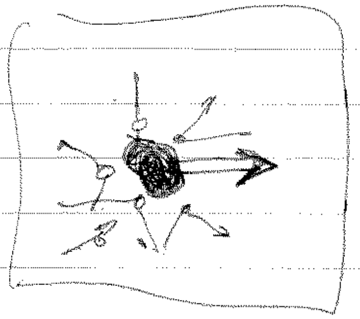


Random impacts of fluid molecules on pollen grain causes Brownian motion and drag

Langevin description (1908)

Eq of motion for Brownian particle

$$\frac{dp}{dt} = F(t) = \langle F(t) \rangle + \mathcal{F}(t)$$

Mean force $F(t) = -\gamma p$ (drag)

$\mathcal{F}(t)$ = Fluctuations $\langle \mathcal{F}(t) \rangle = 0$

$\Rightarrow$ Langevin equation

$$\frac{dp}{dt} = -\gamma p + \mathcal{F}(t)$$

$$\langle \mathcal{F}(t) \rangle = 0$$

$$\langle \mathcal{F}(t)\, \mathcal{F}(t') \rangle = \underset{\substack{\Uparrow \\ \text{convention}}}{2} D\, g(t-t')$$ Stationary state

Correlation time τ_c = range over which $g(\tau)$ is nonnegligible

Here $\tau_c \sim$ Collision time between molecule + grain $\ll \frac{1}{\gamma}$

$$\Rightarrow \langle \mathcal{F}(t)\, \mathcal{F}(t') \rangle \cong 2D\, \delta(t-t')$$ Markov approx.

Formal solution:

$$p(t) = p(t_0)\, e^{-\gamma(t-t_0)} + \int_{t_0}^{t} dt' \, \mathcal{F}(t') \, e^{-\gamma(t-t')}$$

$$\langle p(t) \rangle = p(t_0)\, e^{-\gamma(t-t_0)} \quad \text{drag}$$

$$\langle \Delta p^2(t) \rangle = \langle p^2(t) \rangle - \langle p(t) \rangle^2$$

$$= \langle (p(t) - \langle p(t) \rangle)^2 \rangle$$

$$= \int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' \underbrace{\langle \mathcal{F}(t') \mathcal{F}(t'') \rangle}_{2D\,\delta(t'-t'')} e^{-\gamma(t-t')} e^{-\gamma(t-t'')}$$

$$= 2D \int_{t_0}^{t} dt' \, e^{-2\gamma(t-t')} = \frac{D}{\gamma}\left(1 - e^{-2\gamma(t-t_0)}\right)$$

For $\tau_c \ll t - t_0 \ll \frac{1}{\gamma}$

$$\langle \Delta p^2(t) \rangle = \frac{D}{\gamma}\left(2\gamma(t-t_0)\right) = 2D\,(t-t_0)$$

$\Longrightarrow$ Diffussion: Fluctuations grow linearly in time

For $t - t_0 \gg \frac{1}{\gamma} \Longrightarrow$ Equilibrium

$$\langle \Delta p^2 \rangle_{S.S.} = \langle p^2 \rangle_{S.S.} = \frac{D}{\gamma} \qquad \frac{\langle p^2 \rangle}{2M} = \frac{1}{2} k_B T$$

$$\Longrightarrow D = (M k_B T)\,\gamma$$

Fluctuation-dissipation relation

Other correlation functions ("Einstein Relations")

In the Markov approximation the initial condition is quickly forgotten. Take $t_0 \to -\infty$

$$p(t') = \int_{-\infty}^{t'} dt'' \, \mathcal{F}(t'') \, e^{-\gamma(t'-t'')} \qquad \left(t' \gg \frac{1}{\gamma}\right)$$

$$\Rightarrow \quad \langle p(t') \mathcal{F}(t) \rangle = \int_{-\infty}^{t'} dt'' \, \langle \mathcal{F}(t'') \mathcal{F}(t) \rangle \, e^{-\gamma(t'-t'')}$$

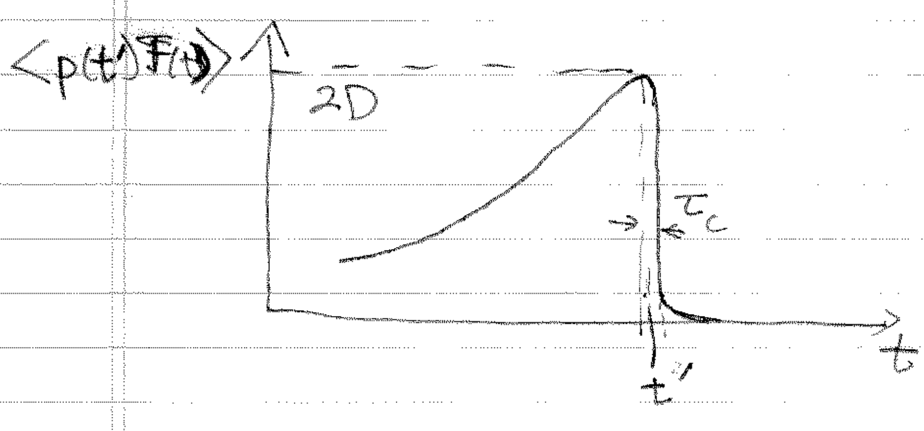
- If $t > t'$ and $t - t' \gg \tau_c$, then since $t'' < t'$
  $t - t'' \gg \tau_c \Rightarrow \langle \mathcal{F}(t'') \mathcal{F}(t) \rangle = 0$

  $$\Rightarrow \quad \langle p(t') \mathcal{F}(t) \rangle = 0 \qquad t - t' \gg \tau_c$$

  ($\mathcal{F}(t)$ in the future of $p(t')$)

- If $t < t'$ and $t' - t \gg \tau_c \Rightarrow t'' - t \gg \tau_c$

  $$\Rightarrow \langle p(t') \mathcal{F}(t) \rangle = 2D \, e^{-\gamma(t'-t)}$$



Correlation between $p(t')$ and $\mathcal{F}(t)$ only for t in the past of t'

Evolution of momentum autocorrelation function

$$\frac{d}{dt}\langle p(t)p(t')\rangle = -\gamma\langle p(t)\,p(t')\rangle + \langle \mathcal{F}(t)\,p(t')\rangle$$

Take t' as the initial condition, $\langle p(t'{=}t)p(t)\rangle = \langle p^2(t)\rangle$

$$\Rightarrow \langle p(t)\,p(t')\rangle = \langle p^2(t)\rangle\, e^{-\gamma|t-t'|} + \underbrace{\int_{t'}^{t} dt'' \,\langle \mathcal{F}(t'')\,p(t')\rangle}_{\leq D\tau_c \;<<\; D\gamma}$$

$\Rightarrow$ In Markov approximation

$$\langle \mathcal{F}(t)\,p(t')\rangle << \gamma\,\langle p(t)\,p(t')\rangle$$

$\therefore\ t \geq t'$ $\boxed{\frac{d}{dt}\langle p(t)\,p(t')\rangle = -\gamma\,\langle p(t)\,p(t')\rangle}$

"Regression theorem": Second order correlation function satisfies same equation of motion as expectation values

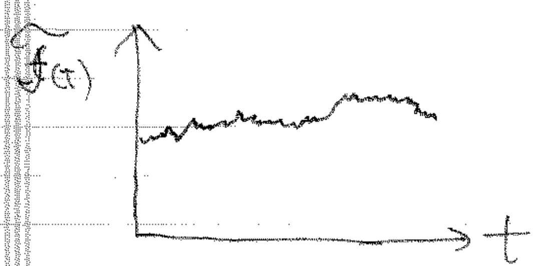
Note: $\int d\tau\, \langle p(\tau)\,p(0)\rangle\, e^{i\omega\tau} = |p(\omega)|^2$ (Power spectrum)

$=$ Lorenzian

Stochastic Differential Equations

The Langenvin equations, as written are physically meaningless. This is important for numerics

To satisfy $\langle \mathcal{F}(t)\,\mathcal{F}(t')\rangle = 2D\,\delta(t-t')$, the fluctuating force must be everywhere nondifferiable (~~it~~ can be continuous)



e.g

Since $\mathcal{F}(t)$ is continous, its integral exists

Define $\mathcal{F}(t) = \sqrt{2D}\,\eta(t)$ $\qquad \langle \eta(t)\,\eta(t')\rangle = \delta(t-t')$

Define $W(t) = \int_{t_0}^{t} \eta(t)\,dt \qquad \frac{dW}{dt} = \eta(t)$

$$\Rightarrow p(t) - p(t_0) = -\gamma\int_{t_0}^{t} p(t')\,dt' + \sqrt{2D}\int_{t_0}^{t} dW(t')$$

$dW(t) \equiv W(t+dt) - W(t)$ = Weiner measure

Properties
Gaussian Random variable
$$\begin{cases} \langle dW(t)\rangle = 0 \\ \langle dW(t)\,dW(t')\rangle = 0 \qquad t \neq t' \\ \langle dW(t)\,dW(t)\rangle = \langle dW^2(t)\rangle = dt \end{cases}$$

Stochastic ~~dif~~ dif'eq

$$\boxed{dp = \underbrace{-\gamma p\,dt}_{\text{Damping}} + \underbrace{\sqrt{2D}\,dW(t)}_{\text{white noise}}}$$

Weiner process ← Gaussian / Markov

Heisenberg - Langevin Equations

Let us return to the quantum description of the damped SHO through the system-reservoir coupling:

$$\hat{H} = \hat{H}_S + \hat{H}_R + \hat{H}_{SR}$$

$$\hat{H}_S = \hbar\omega_0 \hat{a}^\dagger \hat{a} \qquad \hat{H}_R = \sum_j \hbar(\kappa_j \hat{b}_j \hat{a}^\dagger + \kappa_j^* \hat{b}_j^\dagger \hat{a})$$

$$\hat{H}_R = \sum_j \hbar\omega_j \hat{b}_j^\dagger \hat{b}_j$$

Heisenberg equations of motion

$$\frac{d}{dt}\hat{a} = \frac{-i}{\hbar}[\hat{a}, \hat{H}] = -i\omega_0 \hat{a} - i\sum_j \kappa_j \hat{b}_j$$

$$\frac{d}{dt}\hat{b}_j = \frac{-i}{\hbar}[\hat{b}_j, \hat{H}] = -i\omega_j \hat{b}_j - i\sum_j \kappa_j^* \hat{a}$$

$$\hookrightarrow \hat{b}_j(t) = e^{-i\omega_j t}\hat{b}_j(0) - i\kappa_j^* \int_0^t dt'\, e^{-i\omega_j(t-t')}\, \hat{a}(t')$$

Go to rotating frame $\hat{a}(t) \equiv e^{-i\omega_0 t}\tilde{a}(t)$

$$\Rightarrow \dot{\tilde{a}}(t) = -\sum_j |\kappa_j|^2 \int_0^t dt'\, e^{-i(\omega_j-\omega_0)(t-t')}\, \tilde{a}(t') + \hat{\tilde{F}}(t)$$

where $\hat{\tilde{F}}(t) = -i\sum_j \kappa_j \hat{b}_j(0)\, e^{-i(\omega_j-\omega_0)t}$

$\equiv$ Noise operator

Usual Born - Markov approx

$$\sum_j \Rightarrow \int d\omega\, \mathcal{D}(\omega)$$

Density of states

"Broad band"

In Born-Markov $\sum_j |\kappa_j|^2 e^{-i\omega_j(t-t')} \Rightarrow \frac{\Gamma}{2}\delta(t-t') - \underbrace{i\delta\omega}_{\text{shift}}$

$$\Rightarrow \boxed{\begin{aligned} \dot{\tilde{a}} &= -\frac{\Gamma}{2}\tilde{a}(t) + \hat{\mathcal{F}}(t) \\ \langle \hat{\mathcal{F}}^\dagger(t)\,\hat{\mathcal{F}}(t')\rangle_{Res} &= \bar{n}\,\Gamma\,\delta(t-t') \\ \langle \hat{\mathcal{F}}(t)\,\hat{\mathcal{F}}^\dagger(t')\rangle_{Res} &= (\bar{n}+1)\,\Gamma\,\delta(t-t') \end{aligned}}$$

Note $\bar{n} = \frac{1}{e^{\beta\hbar\omega_0} - 1}$ $\quad \beta = \frac{1}{k_B T}$

In high temperature limit $\bar{n} \Rightarrow \frac{k_B T}{\hbar\omega_0} \gg 1$

$$\Rightarrow \langle \mathcal{F}^\dagger(t)\,\mathcal{F}(t')\rangle \cong \langle \mathcal{F}(t)\,\mathcal{F}^\dagger(t')\rangle = \underbrace{\frac{\Gamma}{\hbar\omega_0} k_B T}\ \delta(t-t')$$

Fluctuation-Dissipation. $2D$: Diffusion coef

The Heisenberg eqn's of motion thus take the form of operator versions of the Langevin eqns.

The operator equations must contain ~~to~~ fluctuation source to preserve the commutation relation

$$\tilde{a}(t) = \tilde{a}(0)\,e^{-\frac{\Gamma}{2}t} + \int dt'\, e^{-\frac{\Gamma}{2}(t-t')}\,\hat{\mathcal{F}}(t')$$

$$\Rightarrow [\tilde{a}(t), \tilde{a}^\dagger(t)] = \underbrace{[\tilde{a}(0), \tilde{a}^\dagger(0)]\,e^{-\Gamma t}}_{\text{Decaying fluctuation}} + \underbrace{\int dt'dt''\, e^{+\frac{\Gamma}{2}(t'+t'')}\, e^{-\Gamma t}[\mathcal{F}(t'), \mathcal{F}^\dagger(t'')]}_{\text{Source}}$$

~~Obs~~ Average over reservoir

$$\Rightarrow \langle [\tilde{a}(t), \tilde{a}^\dagger(t)] \rangle_{Res} = e^{-\Gamma t}\Big(\underbrace{[\tilde{a}(0), \tilde{a}^\dagger(0)]}_{=1}$$

$$+ \int dt'\, dt''\, e^{\frac{\Gamma}{2}(t'+t'')} \langle [\hat{\mathcal{F}}(t'), \hat{\mathcal{F}}^\dagger(t'')] \rangle_{Res}$$

Aside: $\langle [\hat{\mathcal{F}}(t'), \hat{\mathcal{F}}(t'')] \rangle_{Res} = \Gamma\, \delta(t'-t'')$

$$\Rightarrow \langle [\tilde{a}(t), \tilde{a}^\dagger(t)] \rangle_{Res} = e^{-\Gamma t}\Big(1 + \Gamma \underbrace{\int_0^t dt'\, e^{\Gamma t'}}_{e^{\Gamma t} - 1}\Big)$$

$$\Rightarrow \boxed{\langle [\tilde{a}(t), \tilde{a}^\dagger(t)] \rangle_{Res} = 1}$$ Commutator preserved

<u>Generalized Einstein relations</u>

$$\frac{d}{dt} \langle \tilde{a}(t) \rangle_{Res} = -\frac{\Gamma}{2} \langle \tilde{a}(t) \rangle_{Res} + \cancel{\langle \hat{\mathcal{F}}(t) \rangle_{Res}}^{\,0}$$

$$\Rightarrow \boxed{\langle \tilde{a}(t) \rangle = e^{-\frac{\Gamma}{2} t} \langle \tilde{a}(0) \rangle}$$

$$\frac{d}{dt} \langle \tilde{a}^\dagger(t)\, \tilde{a}(t) \rangle = -\frac{\Gamma}{2} \langle \tilde{a}^\dagger(t)\, \tilde{a}(t) \rangle + \langle \tilde{a}^\dagger(t)\, \hat{\mathcal{F}}(t) + \hat{\mathcal{F}}^\dagger(t)\, \hat{a}(t) \rangle$$

Aside: $\langle \tilde{a}^\dagger(t)\, \hat{\mathcal{F}}(t) + \hat{\mathcal{F}}^\dagger(t)\, \tilde{a}(t) \rangle = \int_0^t dt' \langle \hat{\mathcal{F}}^\dagger(t')\, \hat{\mathcal{F}}(t) + \hat{\mathcal{F}}^\dagger(t)\, \hat{\mathcal{F}}(t') \rangle\, e^{-\frac{\Gamma}{2}(t-t')}$

$$= \int_{-t}^{t} d\tau\, \underbrace{\langle \hat{\mathcal{F}}^\dagger(t-\tau)\, \hat{\mathcal{F}}(t) \rangle}_{= \bar{n}\, \delta(\tau)}\, e^{-\frac{\Gamma}{2}\tau} = \bar{n}$$

$$\Rightarrow \boxed{\frac{d}{dt} \tilde{n}(t) = -\Gamma \tilde{n}(t) + \bar{n}(\omega_0, T)}$$

Now more generally,

$$\langle \hat{\mathcal{F}}^\dagger(t)\, \hat{a}(t') \rangle = \int_0^{t'} dt'' \langle \hat{\mathcal{F}}^\dagger(t)\, \hat{\mathcal{F}}(t'') \rangle\, e^{-\frac{\Gamma}{2}(t'-t'')}$$

The same reasoning we used classically to approximate this applies here

For $t > t'$ $\hat{\mathcal{F}}^\dagger(t)$ is not correlated with $\hat{a}(t')$ except for a very small interval $t' + \tau_c$

$$\Rightarrow \langle \hat{\mathcal{F}}^\dagger(t)\hat{a}(t') \rangle = \begin{cases} 0 & t > t' + \tau_c \\ 2De^{-t/\tau_c} & t' < t < t' + \tau_c \\ 2De^{+\Gamma(t'-t)} & t < t' \end{cases}$$

Thus, consider $t > t'$

$$\frac{d}{dt}\langle \hat{a}^\dagger(t)\, \hat{a}(t') \rangle = -\frac{\Gamma}{2}\langle \hat{a}^\dagger(t)\, \hat{a}(t') \rangle + \underbrace{\langle \hat{\mathcal{F}}^\dagger(t)\, \hat{b}(t') \rangle}_{\leq D\tau_c}$$

$$\Rightarrow \boxed{\frac{d}{dt}\langle \hat{a}^\dagger(t)\, \hat{a}(t') \rangle \cong -\frac{\Gamma}{2}\langle \hat{a}^\dagger(t)\, \hat{a}(t') \rangle}$$

This is an example of the "Quantum Regression theorem"

M. Lax, Phys. Rev. 145, 110 (1966).

Using the Wiener-Khintchine relation ~~between~~ we can solve for the two time correlator function and find spectra.