Lecture 22: 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 of particles, each undergoing "Brownian motion", under the influence of 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. CIV.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 quantum picture of matter at the turn of the 19th-20th century.
Random impacts of fluid molecular on pollen grain causes Brownian motion and drag.

Langevin description (1908)

Eq of motion for Brownian particle

\[ \frac{dp}{dt} = F(t) = \langle F(t) \rangle + \xi(t) \]

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

\[ \langle \xi(t) \rangle = 0 \]

\[ \langle \xi(t) \xi(t') \rangle = 2D g(t-t') \] \hspace{1cm} \text{Stationary probability}

Correlation time \( \tau_c = \) range over which \( g(t) \) is nonnegligible.

Here \( \tau_c \sim \) Collision time between molecule + grain

\[ \ll \frac{1}{\gamma} \]

\[ \Rightarrow \langle \xi(t) \xi(t') \rangle \approx 2D S(t-t') \] \hspace{1cm} \text{Markov approx.}
Formal solution:

\[ p(t) = p(t_0) e^{-\gamma (t-t_0)} + \int_{t_0}^{t} dt' F(t') e^{-\gamma (t-t')} \]

\[ \langle p(t) \rangle = p(t_0) e^{-\gamma (t-t_0)} \text{ drag} \]

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

\[ = \langle (p(t) - \langle p(t) \rangle)^2 \rangle \]

\[ = \int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' \langle \overline{F(t') F(t'')} \rangle e^{-\gamma (t-t') - \gamma (t-t'')} \]

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

For \( T_c \ll t-t_0 \ll \frac{1}{\gamma} \)

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

\( \Rightarrow \) Diffusion: Fluctuations grow linearly in time

For \( t-t_0 \gg \frac{1}{\gamma} \Rightarrow \) Equilibrium

\[ \langle \Delta p^2 \rangle = \langle p^2 \rangle = \frac{D}{\gamma} \]

\[ \frac{\langle p^3 \rangle}{2m} = \frac{1}{2} k_B T \]

\[ \Rightarrow \ D = \left( \frac{M k_B T}{\gamma} \right) \]

Fluctuation-dissipation relation.
Other correlation functions ("Einstein Relations")

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

\[
p(t') = \int_{-\infty}^{t'} dt'' F(t'') e^{-\beta (t'-t'')} \quad (t' \gg \frac{1}{\lambda})
\]

\[
\Rightarrow \quad \langle p(t') F(t) \rangle = \int_{-\infty}^{t'} dt'' \langle F(t'') F(t) \rangle e^{-\beta (t'-t'')}
\]

- If \( t > t' \) and \( t - t' \gg T_c \), then since \( t'' < t' \)

\[
t - t'' \gg T_c \Rightarrow \langle F(t') F(t) \rangle = 0
\]

\[
\Rightarrow \quad \langle p(t') F(t) \rangle = 0 \quad t - t' \gg T_c
\]

(\( F(t) \) in the future of \( p(t') \))

- If \( t < t' \) and \( t' - t \gg T_c \)

\[
\Rightarrow \quad \langle p(t') F(t) \rangle = 2D e^{-\beta (t' - t)}
\]

\[
\langle p(t') F(t) \rangle
\]

Correlation between \( p(t') \) and \( F(t) \) only for \( t \) in the past of \( t' \)
Evolution of momentum autocorrelation function

\[ \frac{d}{dt} \langle p(t)p(t') \rangle = -\gamma \langle p(t)p(t') \rangle + \langle f(t)p(t') \rangle \]

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

\[ \Rightarrow \langle p(t)p(t') \rangle = \langle p^2(t) \rangle e^{-\gamma |t-t'|} + \int_{t'}^{t} dt'' \langle \dot{f}(t'')p(t') \rangle \]

\[ \leq \Delta E_c << \Delta \gamma \]

\[ \Rightarrow \text{In Markov approximation} \]

\[ \langle \dot{f}(t)p(t) \rangle \ll \gamma \langle p(t)p(t') \rangle \]

\[ \therefore t \gg t' \quad \frac{d}{dt} \langle p(t)p(t') \rangle = -\gamma \langle p(t)p(t') \rangle \]

"Regression theorem": Schwartz-Coleson Correlation function satisfies same equation of motion as expectation values.

\[ \text{Note:} \quad \text{Sdt} \langle p(t)p(0) \rangle e^{i\omega t} = [p(\omega)]^2 \text{ (Power spectrum)} = \text{Lorenzian} \]
Stochastic Differential Equations

The Langevin equations, as written, are physically meaningless. This is important for numerics. To satisfy $\langle F(t) F(t') \rangle = 2D \delta(t-t')$, the fluctuating force must be everywhere nondifferentiable (it can be continuous).

$F(t)$

Since $F(t)$ is continuous, its integral exists.

Define $\eta(t) = \frac{\sqrt{2D}}{\eta(t)}$  

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

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

$\quad dW(t) = W(t + dt) - W(t) = \text{Weiner measure}$

Properties

$\begin{cases}
\langle dW(t) \rangle = 0 \\
\langle dW(t) \, dW(t') \rangle = 0 \quad t \neq t'
\end{cases}$

Gaussian Random variable

$\langle dW(t) \, dW(t) \rangle = \langle dW^2(t) \rangle = dt$

Stochastic diffusion, e.g.

$dp = -\gamma p \, dt + \sqrt{2D} \, dW(t)$

Damping White noise  

Weiner process  

Gaussian / Markov
Heisenberg - Langenwin Equations

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

\[ \hat{H} = \hat{H}_S + \hat{H}_R + \hat{H}_{SR} \]

\[ \hat{H}_S = \hbar \omega_0 \hat{\alpha} \hat{\alpha}^\dagger \]

\[ \hat{H}_R = \sum_j \hbar \omega_j \hat{b}_j \hat{b}_j^\dagger + \sum_j k_j \hat{b}_j^\dagger \hat{b}_j \]

Heisenberg equations of motion

\[ \frac{d}{dt} \hat{\alpha} = -i \frac{\hbar}{\pi} [\hat{\alpha}, \hat{H}] = -i \omega_0 \hat{\alpha} - i \sum_j k_j \hat{b}_j \]

\[ \frac{d}{dt} \hat{b}_j = -i \frac{\hbar}{\pi} [\hat{b}_j, \hat{H}] = -i \omega_j \hat{b}_j - i \sum_j k_j^* \hat{\alpha} \]

\[ \hat{b}_j(t) = e^{-i \omega_j t} \hat{b}_j(0) - i \sum_j k_j^* \int_0^t dt' e^{-i \omega_j (t-t')} \hat{\alpha}(t') \]

Go to rotating frame \( \hat{\alpha}(t) = e^{-i \omega_0 t} \hat{\alpha}(t) \)

\[ \hat{\alpha}(t) = -i \sum_j k_j^2 \int_0^t dt' e^{-i \omega_j (t-t')} \hat{\alpha}(t') + \hat{\Delta}(t) \]

where \( \hat{\Delta}(t) = -i \sum_j k_j \hat{b}_j(0) e^{-i (\omega_j - \omega_0) t} \)

\( \hat{\Delta}(t) = \text{Noise operator} \)

Usual Born - Markov approx

\[ \sum_j \rightarrow \int \text{D}(w) \]

\( \text{Density of states} \)

\( \text{"Broad band"} \)
In Born-Markov, \[ \sum_{j} |\Psi_j|^2 e^{-i\omega_j (t-t')} = \frac{\Gamma}{2} \delta(t-t') - \frac{i\delta\omega}{\hbar} \]

\[ \Rightarrow \quad \dot{\alpha} = -\frac{\Gamma}{2} \alpha(t) + \frac{\Delta}{\hbar} \]

\[ \left\langle \hat{\tilde{F}}(t) \hat{\tilde{F}}(t') \right\rangle_{\text{res}} = \bar{n} \Gamma \delta(t-t') \]

\[ \left\langle \hat{\tilde{F}}(t) \hat{\tilde{F}}(t') \right\rangle_{\text{res}} = (\bar{n} + 1) \Gamma \delta(t-t') \]

Note \( \bar{n} = \frac{1}{e^{\beta \omega_0} - 1} \) \quad \beta = \frac{1}{k_B T} \]

In high temperature limit: \( \bar{n} \approx \frac{k_B T}{\hbar \omega_0} \gg 1 \)

\[ \Rightarrow \quad \left\langle \hat{\tilde{F}}(t) \hat{\tilde{F}}(t') \right\rangle \approx \left\langle \tilde{F}(t) \tilde{F}(t') \right\rangle = \frac{\Gamma}{k_B T} \frac{k_B T}{\hbar \omega_0} \delta(t-t') \]

Fluctuation-Dissipation. 2D: Diffusion of

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

The operator equations must contain both fluctuation and dissipation to preserve the commutation relation

\[ \alpha(t) = \alpha(0) e^{-\frac{\Gamma}{2} t} + \int dt' e^{-\frac{\Gamma}{2} (t+t')} \frac{\Delta}{\hbar} \]

\[ \Rightarrow \quad [\tilde{\alpha}(t), \tilde{\alpha}^+(t')] = [\alpha(0), \alpha^+(0)] e^{-\frac{\Gamma}{2} t} + \int dt'' dt''' e^{\frac{\Gamma}{2} (t+t''+t''')} \delta(t+t''-t''') \]

Decaying fluctuation

Source

Also, average over reservoir
\[
\langle [\hat{a}(t), \hat{a}^+(t)] \rangle_{\text{real}} = e^{-\Gamma t} \left( \frac{1}{2} \left[ \hat{a}(0), \hat{a}^+(0) \right] + \frac{\Gamma}{2} \int dt' e^{\Gamma t'} \langle [\hat{F}(t), \hat{F}(t')] \rangle_{\text{real}} \right)
\]

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

\[
\langle [\hat{a}(t), \hat{a}^+(t)] \rangle_{\text{real}} = e^{-\Gamma t} \left( 1 + \Gamma \int dt' e^{\Gamma t'} \right)
\]

\[
\langle [\hat{a}(t), \hat{a}^+(t)] \rangle_{\text{real}} = 1
\]

Commutator preserved

Generalized Einstein relations

\[
\frac{d}{dt} \langle \hat{a}(t) \rangle_{\text{real}} = -\frac{\Gamma}{2} \langle \hat{a}(t) \hat{a}(t) \rangle_{\text{real}} + \langle \hat{F}(t) \rangle_{\text{real}}
\]

\[
\Rightarrow \langle \hat{a}(t) \rangle = e^{-\frac{\Gamma}{2} t} \langle \hat{a}(0) \rangle
\]

\[
\frac{d}{dt} \langle \hat{a}^+(t) \hat{a}(t) \rangle = -\frac{\Gamma}{2} \langle \hat{a}^+(t) \hat{a}(t) \rangle + \langle \hat{F}^+(t) \hat{F}(t) + \hat{F}(t) \hat{F}^+(t) \rangle_{\text{real}}
\]

Aside:
\[
\langle \hat{F}(t) \hat{F}^+(t') + \hat{F}^+(t) \hat{F}(t') \rangle = \int dt' \langle \hat{F}(t-t') \hat{F}(t) \rangle e^{-\frac{\Gamma}{2} t'}
\]

\[
= \frac{\Gamma}{2} \delta(t-t')
\]

\[
\Rightarrow \frac{d}{dt} \langle \hat{n}(t) \rangle = -\Gamma \langle \hat{n}(t) \rangle + \Gamma \langle \omega_0 \rangle
\]
Now more generally,
\[
\langle \hat{F}(t) \hat{\bar{\alpha}}(t') \rangle = \int_0^{t'} dt'' \langle \hat{\alpha}^+\hat{F}(t'') \hat{F}(t''') \rangle e^{-\frac{1}{2} (t'' - t'')}
\]

The same reasoning we used classically to approximate this applies here.

For \( t > t' \), \( \hat{F}(t) \) is not correlated with \( \hat{\alpha}(t) \) except for a very small interval \( t' + \tau_c \)

\[
\Rightarrow \langle \hat{F}(t) \hat{\bar{\alpha}}(t') \rangle = \begin{cases} 
0 & t > t' + \tau_c \\
2D e^{-\frac{1}{2} \tau_c} (t' < t < t' + \tau_c) \\
(2D) e^{+\pi(t' - t)} & t < t'
\end{cases}
\]

Thus, consider \( t > t' \)

\[
\frac{d}{dt} \langle \hat{\alpha}^+ \hat{\bar{\alpha}}(t') \rangle = -\frac{\hbar}{2} \langle \hat{\alpha}^+ \hat{\alpha}(t) \rangle + \langle \hat{\bar{\alpha}}(t') \hat{\bar{\alpha}}(t') \rangle
\]

\[
\Rightarrow \frac{d}{dt} \langle \hat{\alpha}^+ \hat{\bar{\alpha}}(t') \rangle = -\frac{\hbar}{2} \langle \hat{\alpha}^+ \hat{\alpha}(t') \rangle
\]

This is an example of the "Quantum Regression Theorem".


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