Quantum Langevin Equation

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Modelling a thermal environment: the Quantum Langevin Equation (QLE)

Ford, Kac and Mazur 1965; Caldeira and Leggett 1983; Ford, Lewis and O'Connel 1988

- A thermal environment can be described as an ensemble of coupled harmonic oscillators.
- This model enables to obtain the quantum mechanical counterpart of the Langevin equation for a Brownian particle moving in an external potential.

$$
\begin{aligned}
H &= H_s + H_B \\
H_s &= \frac{p^2}{2m} + U(x) \\
H_B &= \sum_k \left(\frac{P_k^2}{2m_k} + \frac{1}{2} m_k \omega_k^2 (X_k - x)^2 \right),
\end{aligned}
$$

QLE: cont.

Applying the Heisenberg equation of motion, $\mathrm{i}\hbar dA/dt = [A, H]$, to the Hamiltonian H

$$m\ddot{x} + \frac{\partial U}{\partial x} = \sum_k m_k \omega_k^2 (X_k - x),$$

$$\ddot{X}_k + \omega_k^2 X_k = \omega_k^2 x.$$

Solve first the equation for the bath variables $X_k(t)$...

$$\begin{aligned} X_k(t) &= X_k(0)\cos\omega_k(t-t_0) + \dot{X}_k(0)\frac{\sin\omega_k(t-t_0)}{\omega_k} \\ &+ x(t) - x(0)\cos\omega_k(t-t_0) - \int_{t_0}^{t} dt' \dot{x}(t')\cos\omega_k(t-t'), \end{aligned}$$

QLE: cont.

Applying the Heisenberg equation of motion, $\mathbb{i}\hbar dA/dt = [A, H]$, to the Hamiltonian H

$$
\begin{aligned}
& m\ddot{x} + \frac{\partial U}{\partial x} = \sum_k m_k \omega_k^2 (X_k - x), \\
& \ddot{X}_k + \omega_k^2 X_k = \omega_k^2 x.
\end{aligned}
$$

Solve first the equation for the bath variables $X_k(t)$...

$$
\begin{aligned}
X_k(t) &= X_k(0) \cos \omega_k (t - t_0) + \dot{X}_k(0) \frac{\sin \omega_k (t - t_0)}{\omega_k} \\
&+ x(t) - x(0) \cos \omega_k (t - t_0) - \int_{t_0}^{t} dt' \dot{x}(t') \cos \omega_k (t - t'),
\end{aligned}
$$

QLE: cont.

...and insert the solution in the equations for $x(t)$

$$m\ddot{x}(t) + \int_{t_0}^{t} dt'\gamma(t-t')\dot{x}(t') + \partial_x U = \eta(t)$$

$$\gamma(t) = \theta(t)\sum_k m_k\omega_k^2 \cos\omega_k t$$

$$\eta(t) = \sum_k m_k\omega_k^2\left[(X_k(0)-x(0))\cos\omega_k(t-t_0) + \dot{X}_k(0)\frac{\sin\omega_k(t-t_0)}{\omega_k}\right]$$

The bath enters the picture only through the initial values of its variables $X_k(0)$, $\dot{X}_k(0)$, which appear in the *external force* $\eta(t)$

$[X_k(0), \dot{X}_p(0)] = \mathbb{i}\delta_{kp}\hbar/m$

QLE: cont.

We want the bath to describe a thermal environment at temperature T
Assume that the bath variables are initially in equilibrium at temperature T ($k_B = 1$)
Density matrix $\rho_0 = \mathrm{e}^{-\beta \hat{H}_B}/Z$

$$\langle \tilde{X}_k(0) \tilde{X}_p(0) \rangle = \delta_{kp} \frac{\hbar}{2 m_k \omega_k} \coth \frac{\hbar \omega_k}{2T}$$

$$\langle \dot{X}_k(0) \dot{X}_p(0) \rangle = \delta_{kp} \frac{\hbar \omega_k}{2 m_k} \coth \frac{\hbar \omega_k}{2T}$$

$$\langle \tilde{X}_k(0) \dot{X}_p(0) \rangle = -\langle \dot{X}_k(0) \tilde{X}_p(0) \rangle = \delta_{kp} \frac{i\hbar}{2 m_k}$$

$\tilde{X}_k(0) = X_k(0) - x(0)$

QLE: cont.

Density of states
$$N(\omega) = 2\pi \sum_k m_k \omega_k^2 \delta(\omega - \omega_k),$$

Damping
$$\gamma(t) = \theta(t) \int \frac{d\omega}{2\pi} N(\omega) \cos \omega t,$$

commutator and anti-commutator relations

$$[\eta(t), \eta(t')] = -\mathbb{i} \int \frac{d\omega}{2\pi} N(\omega) \hbar\omega \sin \omega(t - t'),$$

$$\langle \{\eta(t), \eta(t')\} \rangle = \int \frac{d\omega}{2\pi} N(\omega) \hbar\omega \cos \omega(t - t') \coth \frac{\hbar\omega}{2T}.$$

correlations of the quantum noise

$$\begin{aligned} \langle \eta(t)\eta(t') \rangle &= \frac{1}{2} \int \frac{d\omega}{2\pi} N(\omega) \hbar\omega \left[\cos \omega(t - t') \coth \frac{\hbar\omega}{2T} - \mathbb{i} \sin \omega(t - t') \right] \\ &= \frac{1}{2} \int \frac{d\omega}{2\pi} N(\omega) \mathrm{e}^{-\mathbb{i}\omega(t-t')} \hbar\omega (1 + \coth(\hbar\omega/2T)) \end{aligned}$$

QLE: cont.

- Setting $N(\omega) = 2\gamma \Rightarrow \gamma(t) = 2\gamma\,\theta(t)\delta(t)$ (Ohmic approximation)
- taking $\hbar \to 0$ (classical limit)

$$[\eta(t), \eta(t')] = 0,$$
$$\left\langle \eta(t)\eta(t') \right\rangle = 2\gamma T \delta(t - t')$$

- Classical Langevin equation with white Gaussian noise η

$$m\ddot{x}(t) + \eta\dot{x}(t) + \partial_x U(x(t)) = \eta(t)$$

see, e.g., *R. Zwanzig, Nonequilibrium Statistical Mechanics (book)*

QLE with a grain of salt

an oscillator in contact with heat bath at temperature T
Equilibrium

$$
\begin{aligned}
H_s &= \frac{1}{2m}p^2 + \frac{m\omega_s^2}{2}x^2 \\
\langle x^2 \rangle &= \frac{\hbar}{2m\omega_s}\coth(\hbar\omega_s/2T).
\end{aligned}
$$

Dynamic
set $f(t) = \int \mathrm{d}\omega/(2\pi)\mathrm{e}^{-\mathbb{i}\omega t} f(\omega)$

$$
\begin{aligned}
m\ddot{x}(t) &= -m\omega_s^2 x(t) - \gamma\dot{x}(t) + \eta(t) \\
x(\omega) &= -\frac{\eta(\omega)}{m(\omega^2 - \omega_s^2) + \mathbb{i}\gamma\omega} \\
\langle \eta(\omega)\eta(\omega') \rangle &= 2\pi\delta(\omega+\omega')\gamma\hbar\omega(1+\coth(\hbar\omega/2T)) \\
\langle x(t)^2 \rangle &= \int \frac{d\omega}{2\pi} \frac{\gamma\hbar\omega\coth(\hbar\omega/2T)}{(m\omega^2 - m\omega_s^2)^2 + (\omega\gamma)^2}
\end{aligned}
$$

QLE with a grain of salt: cont.

$$\langle x(t)^2 \rangle = \int \frac{d\omega}{2\pi} \frac{\gamma\hbar\omega \coth(\hbar\omega/2T)}{(m\omega^2 - m\omega_s^2)^2 + (\omega\gamma)^2}$$

In the upper half complex plane the integral has

- two simple poles at $z_\pm = \frac{1}{2m}(\mathbb{i}\gamma \pm \sqrt{4m^2\omega_s^2 - \gamma^2})$
- an infinite (but isolated) number of poles along the positive complex axis $z_k = 2\pi ikT/\hbar$, $k = 1, 2 \ldots$

The integral will depend on γ too, while we know that the equilibrium value of $\langle x^2 \rangle$ does not

QLE with a grain of salt: cont.

Let's introduce

$$A(\omega) = \frac{m\omega_s^2}{\pi} \frac{\gamma}{(m\omega^2 - m\omega_s^2)^2 + (\omega\gamma)^2}$$

$$\text{with } \int d\omega A(\omega) = 1$$

$$\text{and } A(\omega_s) = m/(\gamma\pi)$$

$$\lim_{\gamma\to 0} A(\omega) = \delta(\omega - \omega_s)$$

We can write

$$\langle x^2 \rangle = \int d\omega \frac{A(\omega)}{2m\omega_s^2} \hbar\omega \coth(\hbar\omega/2T)$$

and

$$\lim_{\gamma\to 0} \langle x^2 \rangle = \lim_{\gamma\to 0} \int d\omega \frac{A(\omega)}{2m\omega_s^2} \hbar\omega \coth(\hbar\omega/2T) = \frac{\hbar}{2m\omega_s} \coth(\hbar\omega_s/2T)$$