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Tutorial II
Zwanzig-Caldeira-Leggett Hamiltonian

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Zwanzig-Caldeira-Leggett Hamiltonian

We study a Hamiltonian modelling of the generalized Langevin equation. It is known in the quantum community as the Caldeira-Leggett Hamiltonian, but as the Zwanzig Hamiltonian among statistical physicists. The original idea dates back to a paper by Ford, Kac and Mazur (*J. Math. Phys., 6, 504*) in 1965. This work is pivotal for at least two reasons : it allows to understand how irreversibility can emerge from a time-symmetric dynamics (by a proliferation of auxiliary degrees of freedom), and it gives a rigorous framework to study many stochastic problems, for instance the correct quantum quantification of the brownian motion.

One considers the dynamics of one degree of freedom x (the generalization to many is straightforward) described by the Hamiltonian

$$\mathcal{H}_s(x,p) = \frac{p^2}{2M} + U(x) \tag{1}$$

This degree of freedom is put in interaction with a thermal bath, modelled by auxiliary degrees of freedom (p_j, r_j) and the coupling Hamiltonian

$$\mathcal{H}_b(r_i, p_i, x) = \sum_{i=1}^{N} \left\{ \frac{p_i^2}{2m} + \frac{1}{2} m\omega_i^2 \left[r_i - \frac{c_i}{m\omega_i^2} x \right]^2 \right\} \tag{2}$$

Equilibrium properties

The total Hamiltonian is $\mathcal{H}_{\text{tot}}(x, p, r_i, p_i) = \mathcal{H}_s + \mathcal{H}_b$. Show that the canonical partition function factorize. Does $\mathcal{H}_b$ modify the equilibrium properties of x ?

$$\begin{aligned} Z &= \frac{1}{h^{N+1}} \int \mathrm{d}x\mathrm{d}p \int \mathrm{d}r_1\mathrm{d}p_1 \cdots \int \mathrm{d}r_N\mathrm{d}p_N \exp(-\beta[H_s + H_b]) \\ &= \frac{1}{h^{N+1}} \left(\int \mathrm{d}p \exp\left(-\frac{\beta p^2}{2M}\right)\right) \left(\prod_{i=1}^{N} \int \mathrm{d}p_i \exp\left(-\frac{\beta p_i^2}{2m}\right)\right) \times \\ &\quad \int \mathrm{d}x\mathrm{d}r_1 \cdots \mathrm{d}r_N \exp\left(-\frac{\beta m}{2} \sum_i \omega_i^2 \left[r_i - \frac{c_i}{m\omega_i^2} x \right]^2 - \beta U(x)\right) \end{aligned}$$

We can make a change of variable,

$$\hat{r}_i = r_i - \frac{c_i}{m\omega_i^2} x, \qquad \mathrm{d}\hat{r}_i = \mathrm{d}r_i$$

$$\int_{-\infty}^{+\infty} \mathrm{d}x \cdots \int_{-\infty}^{+\infty} \mathrm{d}\hat{r}_N \exp\left(-\frac{\beta m}{2} \sum_i \omega_i^2 \hat{r}_i^2 - \beta U(x)\right) = \int_{\mathbb{R}} \mathrm{d}x \exp(-\beta U(x)) \times \prod_i \int_{\mathbb{R}} \mathrm{d}\hat{r}_i \exp\left(-\frac{\beta m}{2} \omega_i^2 \hat{r}_i^2\right)$$

and thus, the paramount important question is, *how does H_b modify the equilibrium properties of x ?*

$$\langle A(x,p)\rangle = \frac{\int \mathrm{d}x\mathrm{d}p \int \mathrm{d}r_j A(x,p)\exp(-\beta[H_s+H_b])}{\int \mathrm{d}x\mathrm{d}p \int \mathrm{d}r_j \exp(-\beta[H_s+H_b])} \to \frac{\int \mathrm{d}x\mathrm{d}p \exp\big(-\beta[p/2M+U(x)]\big)}{\int \mathrm{d}x\mathrm{d}p \exp(-\beta[p^2/2M+U(x)])}$$

Meaning that this coupling doesn't change the properties.

Hamiltonian dynamics

1. Write down the Hamilton equations for (x,p) and the $(r_i,p_i)_s$. Show in particular that

$$\ddot{r}_i + \omega_i^2 r_i = F(t) \tag{3}$$

where F will be given in terms of x and the bath constants (m, ω_i, c_i).

We know hamilton's equation,

$$\begin{cases} \dfrac{\mathrm{d}x}{\mathrm{d}t} = \dfrac{\partial\mathcal{H}}{\partial p} = \dfrac{p}{M} \\ \dfrac{\mathrm{d}p}{\mathrm{d}t} = -\dfrac{\partial\mathcal{H}}{\partial x} \end{cases} \qquad \begin{cases} \dfrac{\mathrm{d}r_i}{\mathrm{d}t} = \dfrac{\partial\mathcal{H}}{\partial p_i} = \dfrac{p_i}{m} \\ \dfrac{\mathrm{d}p_i}{\mathrm{d}t} = -\dfrac{\partial\mathcal{H}}{\partial r_i} \end{cases}$$

$$-p_i' = -mr_i' = m\omega_i^2\left[r_i - \frac{c_i}{m\omega_i^2}x\right]$$

And thus,

$$\ddot{r}_i + \omega_i^2 r_i = \underbrace{\frac{c_i}{m}x(t)}_{F(t)}$$

2. To solve (3), one compute first the *causal Green function* of the equation, namely the function $G(t)$ solution of

$$\ddot{G} + \omega_i^2 G = \delta(t) \tag{4}$$

such that $G(t) = \Theta(t)g(t)$ where Θ is the Heaviside's function, and $g(t)$ a regular function defined over $\mathbb{R}^+$. Find $g(t)$. Why is $G(t)$ termed a *causal* function ?

"causal" because the response $g(t)$ comes after the excitation $\delta(t)$.

$$[\Theta(t)g(t)]'' + \omega_i^2\Theta g = \delta t$$

$$\Theta' = \delta(t), \qquad \Theta'' = \delta'(t)$$

$$\delta'(t)g(t) + 2\delta(t)g'(t) + \Theta g'' + \omega_i^2 \Theta g = \delta(t)$$

we consider strictly positive time and thus,

$$g'' + \omega_i^2 g = 0$$

and thus,

$$g = g_0 \cos \omega_i t + \frac{g_0'}{\omega_i} \sin(\omega_i t)$$

The dynamical equation amounts now to,

$$\delta'(t)g(t) + 2\delta(t)g'(t) = \delta(t)$$

leading to,

$$2g'(0) = 1, \qquad\qquad g(0) = 0$$

$$\delta(t)g(t) = \delta(t)g(0)$$

But,

$$\delta'(t)g(t) \neq \delta'(t)g(0)$$

But instead,

$$\delta'(t)g(t) = \delta'(t)g(0) - \delta(t)g'(0)$$

Thus we have to correct,

$$\delta'(t)g(0) + \delta(t)g'(0) = \delta(t)$$

and now there is no longer any problems, and so, $g'(0) = 1$ and $g(0) = 0$. At the end of the day,

$$G(t) = \Theta \frac{\sin \omega_i t}{\omega_i}$$

3. Check that a particular solution of (3) is $\int_{-\infty}^{+\infty} \mathrm{d}s G(t-s)F(s)$. Show that it yields

$$r_i(t) = r_i(0)\cos(\omega_i t) + \frac{p_i(0)}{m\omega_i}\sin(\omega_i t) + \frac{c_i}{m\omega_i}\int_0^t \mathrm{d}s x(s)\sin[\omega_i(t-s)] \tag{5}$$

Green function method,

$$\ddot{G} + \omega_i^2 G = \delta(t) \longrightarrow G(t) = \Theta(t)\frac{\sin \omega_i t}{\omega_i}$$

$G(t)$ is a powerful tool to solve time-translation invariant linear differential equation by excitation (here $F(t)$).

$$\begin{cases} r_i(t) = \int_{-\infty}^{+\infty} \mathrm{d}s G(t-s)F(s) \\ \dot{r}_i(t) = \int_{-\infty}^{+\infty} \mathrm{d}s G'(t-s)F(s) \\ \ddot{r}_i(t) = \int_{-\infty}^{+\infty} \mathrm{d}s G''(t-s)F(s) \end{cases}$$

Leading to,

$$r_i'' + \omega_i^2 r_i = \int \mathrm{d}s \underbrace{\left[G''(t-s) + \omega_i^2 G(t-s)\right]}_{\delta(t-s)} F(s) = F(t)$$

Reminder :

$$\frac{c_i}{m} x(t) = F(t)$$

The most general solution of Eq. (3) is

$$r_i(t) = A\cos(\omega_i t) + B\sin(\omega_i t) + \underbrace{\int \mathrm{d}s \frac{\sin\omega_i(t-s)}{\omega_i}\Theta(t-s)\left(\frac{c_i}{m}\right)x(s)}_{\frac{c_i}{m\omega_i}\int_{-\infty}^{t}\mathrm{d}s\sin\omega_i(t-s)x(s)}$$

$$r_i(t) = A\cos\omega_i t + B\sin\omega_i t + \frac{c_i}{m\omega_i}\int_{-\infty}^{0}\mathrm{d}s\sin\omega_i(t-s)x(s) + \frac{c_i}{m\omega_i}\int_{0}^{t}\mathrm{d}s\sin\omega_i(t-s)x(s)$$

we can transform in the $\int_{-\infty}^{0}$,

$$\frac{c_i}{m\omega_i}\int_{-\infty}^{0}\mathrm{d}s\sin\omega_i(t-s)x(s) = \frac{c_i}{m\omega_i}\sin\omega_i t \times \mathrm{cst}$$

which can be integrated in the B term. Thus,

$$r_i(t) = \tilde{A}\cos\omega_i t + \tilde{B}\sin\omega_i t + \frac{c_i}{m\omega_i}\int_{0}^{t}\mathrm{d}s\sin\omega_i(t-s)x(s)$$

at $t=0$, $r_i(0) = \tilde{A}$,

$$\dot{r}_i(0) = +\omega_i\tilde{B} + \frac{c_i}{m\omega_i}\sin(\omega_i(t-t))x(t) + \frac{c_i}{m\omega_i}\int_{0}^{0}\mathrm{d}s\omega_i\cos\omega_i(t-s)x(s) = \omega_i\tilde{B}$$

and so,

$$\begin{cases} \tilde{A} = r_i(0) \\ \tilde{B} = \dfrac{v_i(0)}{\omega_i} = \dfrac{p_i(0)}{m\omega_i} \end{cases}$$

4. Show also that for all $\tau > 0$,

$$r_i(t) = r_i(-\tau)\cos(\omega_i(t+\tau)) + \frac{p_i(-\tau)}{m\omega_i}\sin(\omega_i(t+\tau)) + \frac{c_i}{m\omega_i}\int_{-\tau}^{+t} \mathrm{d}s x(s)\sin[\omega_i(t-s)] \quad (6)$$

Same as before but now the integral split up in,

$$\int_{-\infty}^{+\infty} \longrightarrow \int_{-\infty}^{-\tau} + \int_{-\tau}^{+\infty}$$

Generalized Langevin Equation

5. By integrating by parts the last term of (5), show that the dynamical equation of x can be written

$$\dot{p} = -\frac{\mathrm{d}U}{\mathrm{d}x} - \int_0^t \mathrm{d}s\zeta(t-s)\frac{p(s)}{M} + F_B(t) \quad (7)$$

where the explicit expressions of $\zeta(t)$ (friction kernel) and $F_B(t)$ (noise, random force) will be given.

$$r_i(t) = r_i(0)\cos\omega_i t + \frac{p_i(0)}{m\omega_i}\sin\omega_i t + \frac{c_i}{m\omega_i}\left[\left[x(s)\frac{\cos(\omega_i(t-s))}{\omega_i}\right]_0^t - \frac{1}{\omega_i}\int_0^t \mathrm{d}s\dot{x}(s)\cos(\omega_i(t-s))\right]$$

$$= \left[r_i(0) - \frac{c_i x(0)}{m\omega_i}\right]\cos\omega_i t + \frac{p_i(0)}{m\omega_i}\sin\omega_i t + \frac{c_i}{m\omega_i^2}x(t) - \frac{c_i}{m}\int_0^t \mathrm{d}s\dot{x}(s)\cos\omega_i(t-s)$$

We remind that,

$$\dot{x} = \frac{\partial\mathcal{H}}{\partial p} = \frac{p}{M}$$

$$\dot{p} = -\frac{\partial\mathcal{H}}{\partial x} = -U'(x) + \sum_i \frac{c_i m\omega_i^2}{m\omega_i^2}\left[r_i - \frac{c_i}{m\omega_i^2}x\right] = -U'(x) + \sum_{j=1}^{N} c_j\left[r_j - \frac{c_j x}{m\omega_j^2}\right]$$

$$\dot{p} = -U'(x) + \underbrace{\sum_j c_j\left\{\left[r_i(0) - \frac{c_i x(0)}{m\omega_i}\right]\cos\omega_i t + \frac{p_i(0)}{m\omega_i}\sin\omega_i t\right\}}_{F_B(t)} - \int_0^t \mathrm{d}s\frac{p(s)}{M}\underbrace{\left(\sum_{j=1}^{N}\frac{c_j^2}{m\omega_j^2}\cos\omega_j(t-s)\right)}_{=\zeta(t-s)}$$

we see that we have some initial condition $r_i(0)$, $x(0)$ and $p_i(0)$.
Leading to a generalized Langevin equation,

$$\dot{p} = -\frac{\mathrm{d}U}{\mathrm{d}x} - \int_0^t \mathrm{d}s\zeta(t-s)\frac{p(s)}{M} + F_B(t)$$

There is a necessary link between ζ and F_B that Einstein taught us : fluctuation-dissipation.

6. The system is prepared at $t = 0$ by constraining $(x(0), p(0))$ but leaving the bath's degrees of freedom (r_i, p_i) thermalize at temperature T. What is the probability distribution of the (r_i, p_i) ?

$$\mathrm{prob}(r_i, p_i) \propto \exp(-\beta \mathcal{H}_b(r_i, p_i, x(0)))$$

7. One reminds that a Gaussian distribution is given by $p(x) \propto \exp(-(x-\bar{x})^2/[2\sigma^2])$ where $\bar{x}$ is the average of the variable and $\sigma^2 = \bar{x^2} - (\bar{x})^2$ its variance. Show without calculations that

$$\langle F_B(t) \rangle = 0 \tag{8}$$
$$\langle F_B(t) F_B(t') \rangle = k_B T \zeta(t - t') \tag{9}$$

where the meaning of the average brackets will be precised.

$$\langle F_B(t) \rangle = \sum_i c_j \left[\left\langle r_i(0) - \frac{c_i x(0)}{m\omega_i} \right\rangle \cos\omega_i t + \left\langle \frac{p_i(0)}{m\omega_i} \right\rangle \sin\omega_i t \right] = 0$$

What is $\langle \cdots \rangle$? this correspond to at time $t = 0$, fixing initial conditions, sorting out the the values of r_i and p_i from the distribution given in question 6. $\langle \cdot \rangle$ corresponds to sampling p_j and r_j according to the gaussian distribution of q6, being always taken at the same fixed time.

$$\langle F_B(t) F_B(t') \rangle = \sum_j \sum_{j'} c_j c_{j'} \left\{ \langle \tilde{r}_j \tilde{r}_{j'} \rangle \cos\omega_j t \cos\omega_j t' + \left\langle \frac{p_j p_{j'}}{m^2 \omega_j \omega_{j'}} \right\rangle \sin\omega_j t \sin\omega_{j'} t' + \right.$$
$$\left. \left\langle \frac{\tilde{r}_j p_{j'}}{m\omega_{j'}} \right\rangle \cos\omega_j t \sin\omega_{j'} t' + \left\langle \frac{\tilde{r}_{j'}}{m\omega_j} p_j \right\rangle \cos\omega_{j'} t' \sin\omega_j t \right\}$$

The red part is equal to 0 because the gaussian distribution doesn't couple $\tilde{r}_j$ ad $p_{j'}$. The green part is equivalent to $\langle \tilde{r}_{j'} \rangle \langle p_j \rangle$ which is equal to 0.

$$\langle \tilde{r}_j \tilde{r}_{j'} \rangle = \begin{cases} j \neq j' \implies = 0 \\ j = j' \implies = \langle \tilde{r}_j^2 \rangle = \dfrac{k_B T}{m\omega_j^2} \end{cases}$$

$$\langle \tilde{p}_j \tilde{p}_{j'} \rangle = \begin{cases} j \neq j' \implies = 0 \\ j = j' \implies = m k_B T \end{cases}$$

And finally,

$$\begin{aligned}\langle F_B(t)F_B(t')\rangle &= \sum_j c_j^2\left[\frac{k_BT}{m\omega_j p2}\cos\omega_j t\cos\omega j t' + \frac{mk_BT}{m^2\omega_j^2}\sin\omega_j t\sin\omega_j t'\right]\\ &= k_BT\sum_j\frac{c_j^2}{m\omega_j^2}\cos\omega_j(t-t')\\ &= k_BT\zeta(t-t')\end{aligned}$$

which the fluctuation dissipation theorem of the second kind. The noise correlation is time translation invariant.

8. The equation (9) is called a *fluctuation-dissipation relation.* Why ?

A variant

The preceding definition of the noise and its statistical properties is a little problematic, because the statistical distribution of the thermal degrees of freedom depends on $(x(0), p(0))$, the initial characteristic of the process. To overcome this problem, the generalized Langevin equation can be slightly rewritten.

9. Show that the dynamical equation of $x(t)$ can be also expressed as

$$\dot{p} = -\frac{\mathrm{d}U}{\mathrm{d}x} - \int_{-\tau}^{+t}\mathrm{d}s\zeta(t-s)\frac{p(s)}{M} - x(-\tau)\zeta(t+\tau) + \tilde{F}_B(t) \tag{10}$$

where $\tilde{F}_B(t)$ will be precised in terms of the $(r_i(-\tau), p_i(-\tau))$.

Clearly Eq. (6) is involved,

$$\dot{p} = -U'(x) + \sum_j c_j\left[r_j - \frac{c_j}{m\omega_j^2}x\right]$$

Eq. (6) becomes,

$$r_i(t) = r_i(-\tau)\cos\omega_i(t+\tau) + \frac{p_i(-\tau)}{m\omega_i}\sin(\omega_i(t+\tau)) + \frac{c_i}{m\omega_i}\left(\left[x(s)\frac{\cos\omega_i(t-s)}{\omega_i}\right]_{-\tau}^{t} - \frac{1}{\omega_i}\int_0^t\mathrm{d}s\dot{x}(s)\cos\omega_i(t-s)\right)$$

$$\left[r_i(-\tau) - \frac{c_i}{m\omega_i^2}x(-\tau)\right]\cos\omega_i(t+\tau) + \frac{p_i(-\tau)}{m\omega_i}\sin(\omega_i(t+\tau)) + \frac{c_i}{m\omega_i^2}x(t) - \frac{c_i}{m\omega_i^2}\int_{-\tau}^t\mathrm{d}s\dot{x}(s)\cos\omega_i(t-s)$$

thus,

$$\dot{p} = -U'(x) + \sum_j c_j\left\{\left[r_j(-\tau)\cos\omega_j(t+\tau) + \frac{p_j(-\tau)}{m\omega_j}\sin(\omega_j(t+\tau))\right] - \frac{c_j}{m\omega_j^2}x(-\tau)\cos\omega_j(t+\tau) - \frac{c_j}{m\omega_j^2}\int_{-\tau}^t\cdots\right\}$$

Thus,

$$\dot p = -U'(x) + \tilde F_B - x(-\tau)\underbrace{\left(\sum_j \frac{c_j^2}{m\omega_j^2}\cos\omega_j(t+\tau)\right)}_{=\zeta(t+\tau)} - \int_{-\tau}^{t} \mathrm{d}s\dot x(s)\underbrace{\left(\sum_j \frac{c_j^2}{m\omega_j^2}\cos\omega_j(t-s)\right)}_{=\zeta(t-s)}$$

$$\tilde F_B(t) = \sum_j c_j\left[r_j(-\tau)\cos\omega_j(t+\tau) + \frac{p_j(-\tau)}{m\omega_j}\sin\omega_j(t+\tau)\right]$$

By choosing carefully (c_j, m, ω_j) we can emulate whatever $\zeta(t)$ we desire.

10. Assuming that $t > 0$ and that $\zeta(t) \to 0$ when $t \to \infty$, give the limiting for of the preceding equation when $\tau \to \infty$.

when $\tau \to +\infty$, which is equivalent to the time at which we prepared the system $(-\tau)$ is thrown in infinitely remote past), meaning we can forget $\zeta(t+\tau)$, $x(-\tau)$ is forgotten.

$$\dot p = -U'(x) + \tilde F_B - \int_{-\infty}^{t} \mathrm{d}s\dot x(s)\zeta(t-s)$$

Now, $\tilde F_B(t)$ is differently defined, as well as $\langle\cdots\rangle$,

$$\text{prob}(r_i(-\tau), p_j(-\tau)) \propto \exp(-\beta\mathcal{H}(x=0, p=0, r_j(-\tau), p_j(-\tau)))$$

- $$\langle\tilde F_B(t)\rangle = 0$$
- $$\langle\tilde F_B(t)\tilde F_B(t')\rangle = k_B T\zeta(t-t')$$
- Now $\tilde F_B$ is now totally independent from (x, p).

11. Show that (8) and (9) are still valid with $\tilde F_B$, provided the meaning of $\langle\cdots\rangle$ be redefined.

White noise limit

We assume that $\zeta(t)$ goes to zero within a characteristic time τ_ζ and that $\tau_\zeta \ll \tau_p = M/\int_0^{+\infty}\mathrm{d}s\zeta(s)$.

12. What does represent τ_p ?

We know that for an equation,

$$M\dot v = -\gamma v$$

the characteristic relaxation time is $M\gamma^{-1} \equiv \tau_v$ (or written τ_p).

13. Show that the generalized Langevin equation can be approximated by an ordinary Langevin equation.

If $\tau_\zeta \ll \tau_v$ and if we are interested in dynamics of v on frequencies $\geq \tau_v$, then we are blind with respect to the dynamical details brought by $\zeta(v)$. In this case,

$$\int_0^t \mathrm{d}s\zeta(t-s)v(s) \sim \int_0^t \mathrm{d}s\zeta(t-s)v(t) \sim v(t)\int_0^{+\infty} \mathrm{d}s\zeta(s)$$

where $\zeta(t-s)$ is quickly varying and for $t \geq \tau_\zeta$. Since $t \geq \tau_\zeta$, we can go up to $+\infty$ and thus in this case we are back at the ordinary Langevin equation.
But, do not forget to make the white noise in parallel ! Modify also $F_B(t)$ if $\int_t \mathrm{d}s\zeta(t-s)v(s)$ has been touched, we need to respect fluctuation dissipation.
Detailed balance is important in a stochastic model. Fluctuation-dissipation has to be obeyed when interacting with the bath/thermostat.
And pay attention to the "a posteriori" check of the White Noise hypothesis.