Fluctuation-Dissipation Theorem (FDT)

NGL

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Abstract

This is a short writeup with derivation of fluctuation-dissipation theorem (FDT) in classical and quantum mechanics.

1 Classical mechanics

We use Lecture 21 from `http://www.nyu.edu/classes/tuckerman/stat.mech/`.

Liouville equation for $f(\Gamma, t)$, $\Gamma = (q, p)$:

$$\frac{\partial f}{\partial t} + iLf = 0 \tag{1}$$

where $iL = \{\ldots, H\}$ is the Poisson bracket. Consider a small perturbation to a stationary Hamiltonian H_0 and a steady-state distribution $f_0(\Gamma) = e^{-H_0(\Gamma)/T}/Z$:

$$\begin{aligned} H(\Gamma, t) &= H_0(\Gamma) - X(\Gamma)F(t) && (2) \\ iL &= iL_0 + i\Delta L && (3) \\ f(\Gamma, t) &= f_0(\Gamma) + \Delta f(\Gamma, t) && (4) \end{aligned}$$

Let us find Δf using perturbation theory to the first order. We have

$$\left(\frac{\partial}{\partial t} + iL_0\right) \Delta f(\Gamma, t) = -i\Delta L f_0(\Gamma) \tag{5}$$

since $iL_0 f_0 = 0$. Consider the left-hand side:

$$-i\Delta L f_0(\Gamma) = \{f_0, XF(t)\} = F(t)\{f_0, X\} \tag{6}$$

Since $f_0(\Gamma) = e^{-H_0(\Gamma)/T}/Z$,

$$\nabla_\Gamma f_0 = \frac{df_0}{dH_0}\nabla_\Gamma H_0 \tag{7}$$
$$\{f_0, X\} = \frac{df_0}{dH_0}\{H_0, X\} = \frac{1}{T}f_0\left(\frac{dX}{dt}\right)_0 \tag{8}$$

where ∇_Γ denotes a vector consisting of $\partial/\partial q_i$ and $\partial/\partial p_i$ and the subscript "0" denotes time evolution according to unperturbed Hamiltonian H_0. Thus, denoting $\dot{X}(\Gamma) = (dX/dt)_0$, we have

$$-i\Delta L f_0(\Gamma) = \frac{1}{T}F(t)f_0\dot{X} \tag{9}$$

The solution of equation (5) is

$$\begin{aligned}\Delta f(\Gamma, t) &= -\int_0^t dt' e^{-iL_0(t-t')} i\Delta L(t') f_0(\Gamma) \\ &= \frac{1}{T}\int_0^t dt' e^{-iL_0(t-t')} F(t') f_0(\Gamma)\dot{X}(\Gamma)\end{aligned} \tag{10}$$

Consider operator $A(\Gamma)$ and let us find its perturbed average value using the found perturbation Δf:

$$\begin{aligned}\langle A(t)\rangle &= \int d\Gamma A(\Gamma) f(\Gamma, t) = \langle A\rangle_0 + \int d\Gamma A(\Gamma)\Delta f(\Gamma, t) \\ &= \langle A\rangle_0 + \frac{1}{T}\int_0^t dt' F(t') \int d\Gamma A(\Gamma) e^{-iL_0(t-t')} f_0(\Gamma)\dot{X}(\Gamma)\end{aligned} \tag{11}$$

Now we use some trickery with operators: $A(t) = e^{iLt}A(0)$ therefore $A^*(t) = A^*(0)e^{-iLt}$ therefore $A(t) = A(0)e^{-iLt}$. We used the fact that A is real and L is hermitian (why ?). We get

$$\langle A(t)\rangle = \langle A\rangle_0 + \frac{1}{T}\int_0^t dt' F(t') \int d\Gamma_0 A(\Gamma_{t-t'}(\Gamma_0))\dot{X}(\Gamma_0) \tag{12}$$

where $\Gamma_{t-t'}(\Gamma_0)$ is the phase coordinates propagated through time $t - t'$ using H_0.

$$\langle A(t)\rangle = \langle A\rangle_0 + \frac{1}{T}\int_0^t dt' F(t') \langle A(t-t')\dot{X}(0)\rangle_0 \tag{13}$$

The response function

$$\alpha_{AX}(\tau) = \frac{1}{T}\langle A(\tau)\dot{X}(0)\rangle_0 = -\frac{1}{T}\frac{d}{d\tau}\langle A(\tau)X(0)\rangle_0 \tag{14}$$

—valid only for $\tau > 0$. In the last equation we used

$$\frac{d}{dt}\langle A(\tau+t)X(t)\rangle_0 = 0 = \langle \dot{A}(\tau+t)X(t)\rangle_0 + \langle A(\tau+t)\dot{X}(t)\rangle_0 \tag{15}$$

From now on, we drop subscript "0". The linear response is described by

$$\alpha_{AB}(t) = -\frac{1}{T}\frac{d}{dt}\langle A(t)B(0)\rangle \tag{16}$$

If $A \equiv X$, then $\alpha(\tau) = -\frac{1}{T}\frac{d}{d\tau}\langle X(\tau)X(0)\rangle$, the response function is related to the correlation of X. Taking Fourier transforms and using Wiener-Khintchine relation:

$$(X^2)_\omega \equiv \int_{-\infty}^{+\infty} \langle X(\tau)X(0)\rangle e^{i\omega\tau} d\tau = 2\mathrm{Re}\int_0^{+\infty} \langle X(0)X(\tau)\rangle e^{i\omega\tau} d\tau \tag{17}$$

and

$$\begin{aligned}\alpha(\omega) &= \int_{-\infty}^{+\infty} \alpha(\tau) e^{i\omega\tau} d\tau = -\frac{1}{T}\int_0^{+\infty} \frac{d}{d\tau}\langle X(\tau)X(0)\rangle e^{i\omega\tau} d\tau \\ &= \frac{1}{T}\left(\langle X^2\rangle - \langle X\rangle^2 e^{i\omega\infty}\right) + \frac{i\omega}{T}\int_0^{+\infty} \langle X(\tau)X(0)\rangle e^{i\omega\tau} d\tau \\ &= \frac{1}{T}\langle X^2\rangle + \frac{i\omega}{2T}(X^2)_\omega - \frac{\omega}{T}\mathrm{Im}\int_0^{+\infty} \langle X(0)X(\tau)\rangle e^{i\omega\tau} d\tau \end{aligned} \tag{18}$$

For $\omega = 0$ we have

$$\alpha(\omega = 0) = \frac{1}{T}\left(\langle X^2\rangle - \langle X\rangle^2\right) = \frac{\langle(\delta X)^2\rangle}{T} \tag{19}$$

The FDT is the imaginary part of the previous equation

$$\mathrm{Im}\,\alpha(\omega) = \frac{\omega}{2T}(X^2)_\omega \tag{20}$$

or

$$(X^2)_\omega = \frac{2T}{\omega}\mathrm{Im}\,\alpha(\omega) \tag{21}$$

We can consider the fluctuations in X to be caused by random force F. Using $(X^2)_\omega = |\alpha(\omega)|^2 (F^2)_\omega$, we obtain

$$(F^2)_\omega = \frac{2T}{\omega} \frac{\operatorname{Im} \alpha(\omega)}{|\alpha(\omega)|^2} = \frac{2T}{\omega} \operatorname{Im} \left(\frac{1}{\alpha^*(\omega)} \right) \tag{22}$$

Note that this force is ficticious (however, it can be very real — see Example in Section 2.1 below).

Note that is usually applied to dissipative systems. The conservative Hamiltonian H_0 belongs to a super-system with conserved energy, and the dissipative system is just a part of it (see the abovementioned example).

For space-dependent response, $\alpha(\mathbf{r}, t)$, treat spatial coordinate as an index, e.g. $X(\mathbf{r}, t) \equiv A(t)$, $X(0, t) \equiv B(t)$.

$$\alpha(\mathbf{r}, t) = -\frac{1}{T} \frac{d}{dt} \langle X(\mathbf{r}, t) X(0, 0) \rangle \tag{23}$$

2 Examples in classical mechanics

2.1 Damped 1D oscillator

Consider a driven oscillator of mass M at frequency ω_0, with damping force $-\nu p$. The equation of motion is

$$M\ddot{X} = -M\omega_0^2 X - M\nu\dot{X} + F(t) \tag{24}$$

or, in frequency domain,

$$X(\omega) = \alpha(\omega) F(\omega) \tag{25}$$

where

$$\alpha(\omega) = \frac{1}{M(\omega_0^2 - \omega^2 - i\omega\nu)} \tag{26}$$

The spectrum of the force is

$$(F^2)_\omega = \frac{2T}{\omega} \operatorname{Im} \left(\frac{1}{\alpha^*(\omega)} \right) = 2TM\nu \tag{27}$$

The force is delta-correlated, which could be due, e.g., to bombardment by point particles. Let us obtain this result from microscopic consideration by deriving an expression for ν. Assume that the oscillator has transverse area A and is immersed in a gas of density N, temperature T and consisting of molecules of mass $m \ll M$. The hamiltonian H_0 describes the system which includes both the oscillator and the gas, so there is no total energy loss. Assume, however, that there is so much gas that the temperature of the gas does not change as the energy is transfered from oscillator to the gas.

Momentum transfered by a single particle is $\Delta p = 2mv$. The number of particles of velocity v falling on the oscillator surface in unit time is $\lambda(v) = Avf(v)dv$, so that the average force is $2Amv^2 f(v)dv$. The velocity has to be positive for particles falling from the left, and negative for particles falling from the right. Assume the oscillator has velocity V. Then the distribution that it sees is

$$f(v) = \frac{N}{\sqrt{2\pi}v_t} e^{-\frac{(v-V)^2}{2v_t^2}} \approx \frac{N}{\sqrt{2\pi}v_t}\left(1 + \frac{vV}{v_t^2}\right) e^{-\frac{v^2}{2v_t^2}} \tag{28}$$

where $v_t = \sqrt{T/m}$ and we expanded the exponent in a series and neglected terms $O(V^2/v_t^2) \sim m/M$ (we anticipate that V will be of the order of thermal velocity $\sqrt{T/M}$). We use

$$\int_0^\infty v^n e^{-\frac{v^2}{2v_t^2}}\, dv = 2^{n/2} v_t^{n+1} \Gamma\left(\frac{n+1}{2}\right) \tag{29}$$

The average force from particles falling from the left side is

$$\begin{aligned} F_{\text{side}}(V) &= 2Am \int_0^\infty v^2 f(v) dv \\ &= \frac{2NAm}{\sqrt{2\pi}v_t} \int_0^\infty v^2 \left(1 + \frac{vV}{v_t^2}\right) e^{-\frac{v^2}{2v_t^2}} dv \\ &= \frac{2NAm}{\sqrt{2\pi}v_t}\left(\frac{\sqrt{2\pi}v_t^3}{2} + 2\sqrt{2}Vv_t^2\right) \end{aligned} \tag{30}$$

The total force is

$$F(V) = F_{\text{side}}(V) - F_{\text{side}}(-V) = \frac{8NAmVv_t}{\sqrt{\pi}} \tag{31}$$

so that

$$\nu = \frac{8NAmv_t}{\sqrt{\pi}M} = \frac{8NA}{M}\sqrt{\frac{mT}{\pi}} \tag{32}$$

Let us find independently the spectrum of the delta-correlated random force due to bombardment by particles. Spectrum due to particles with velocity v is $(dF^2)_\omega = (\Delta p)^2\lambda(v) = (2mv)^2 Avf(v)dv$. Force due to particles falling from the left and from the right has the spectrum

$$\begin{aligned}
(F^2)_\omega &= 2\int_0^\infty (dF^2)_\omega = 2\int_0^\infty (2mv)^2 Avf(v)dv \\
&= \frac{8NAm^2}{\sqrt{2\pi}v_t}\int_0^\infty v^3 e^{-\frac{v^2}{2v_t^2}}dv = \frac{16NAm^2v_t^3}{\sqrt{\pi}} \\
&= \frac{16NATmv_t}{\sqrt{\pi}} \qquad (33)
\end{aligned}$$

We see that $(F^2)_\omega = 2MT\nu$, as expected.

2.2 Johnson-Nyquist noise

Consider an open circuit consisting of an impedance $Z(\omega)$ (we use physics notation $i = -j$, $\sim e^{-i\omega t}$ in this example). The change in energy due to fluctuations of voltage and charge at ends of the impedance is $\Delta H(t) = -QV(t)$, where voltage plays the role of the external force. Ohm's law is $Q(\omega) = \alpha(\omega)V(\omega)$, where $\alpha(\omega) = i/(\omega Z(\omega))$. Thus, the spectrum is

$$(Q^2)_\omega = \frac{2T}{\omega}\mathrm{Im}\left(\frac{i}{\omega Z}\right) \qquad (34)$$

$$(V^2)_\omega = \frac{2T}{\omega}\mathrm{Im}\,[i\omega Z^*(\omega)] = 2T\mathrm{Re}\,Z(\omega) \qquad (35)$$

The experimentally measured spectrum per unit frequency f is $2(V^2)_\omega$, which is $4T\mathrm{Re}\,Z(\omega)$. The current spectrum is

$$(I^2)_\omega = (V^2)_\omega/|Z(\omega)|^2 = 2T\mathrm{Re}\,(1/Z^*(\omega)) \qquad (36)$$

3 Quantum mechanics

Use Lecture 23 from the same lecture notes (too lazy to copy them, I use classical mechanics mostly anyway).