ICFP M2 – Selected Topics in Statistical Field Theory
TD n° 5 – Stochastic Thermodynamics

Kay Wiese & Camille Aron

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Let us consider a particle of mass m subject to a deterministic, possibly time-dependent, force f and in contact with a thermal bath at temperature $T \equiv 1/\beta$. The dynamics of its position (here in 1d) is described by the Langevin equation

$$m\frac{\mathrm{d}^2 x(t)}{\mathrm{d}t^2} = f(x(t),t) \underbrace{-\eta\frac{\mathrm{d}x(t)}{\mathrm{d}t} + \xi(t)}_{f_{\text{bath}}}, \tag{1}$$

where $\eta \geq 0$ is a friction coefficient and $\xi(t)$ is a Gaussian white noise: $\langle\xi(t)\rangle = 0$ and $\langle\xi(t)\xi(t')\rangle = 2\eta T\delta(t-t')$ where $\langle\ldots\rangle$ indicates the average over the noise realizations. At the initial time $t = -t_0$, the particle is prepared in thermal equilibrium at temperature T_0 in a confining potential $V(x)$, *i.e.* the initial probability distribution is $P(x,\dot{x};-t_0) = \mathcal{Z}^{-1}\exp\left[-\mathcal{E}(x,\dot{x})/T_0\right]$ with the energy $\mathcal{E}(x,\dot{x}) \equiv \frac{1}{2}m\dot{x}^2 + V(x)$ and the corresponding partition function $\mathcal{Z}$.

A – Linear response in the MSR formalism

The probability of a given trajectory $[x(t), t = -t_0 \ldots t_0]$ is expressed in the MSR formalism as a Gaussian path-integral over an auxiliary field $\hat{x}$ (here taken to be real),

$$P[x]\mathcal{D}[x] = \mathcal{D}[x]\int \mathcal{D}[\hat{x}]\mathrm{e}^{-\mathcal{S}[x,\hat{x}]}, \tag{2}$$

where $\mathcal{S}[x,\hat{x}]$, the MSR action functional, can be decomposed into $\mathcal{S}[x,\hat{x}] = \mathcal{S}_{\text{syst}}[x,\hat{x}] + \mathcal{S}_{\text{bath}}[x,\hat{x}]$ with

$$\mathcal{S}_{\text{syst}}[x,\hat{x}] = \ln\mathcal{Z} + \mathcal{E}(x(-t_0),\dot{x}(-t_0))/T_0 + \int_{-t_0}^{t_0}\mathrm{d}t\ \mathrm{i}\hat{x}(t)\left[m\partial_t^2 x(t) - f(x(t),t)\right], \tag{3}$$

$$\mathcal{S}_{\text{bath}}[x,\hat{x}] = \eta\int_{-t_0}^{t_0}\mathrm{d}t\ \mathrm{i}\hat{x}(t)\left[\partial_t x(t) - T\mathrm{i}\hat{x}(t)\right]. \tag{4}$$

(1) Show that the two-time correlation function is expressed in the MSR formalism as

$$C(t,t') \equiv \langle x(t)x(t')\rangle = \langle x(t)x(t')\rangle_{\mathcal{S}}, \tag{5}$$

where $\langle\ldots\rangle_{\mathcal{S}}$ indicates the path-integral average $\int\mathcal{D}[x,\hat{x}]\ldots\mathrm{e}^{-\mathcal{S}[x,\hat{x}]}$.

(2) Kubo formula. Show that the linear response of the average position to a prior perturbation $f \to f + \delta f$ can be expressed as the following two-time correlation function

$$R(t,t') \equiv \frac{\delta\langle x(t)\rangle}{\delta f(t')} = \langle x(t)\mathrm{i}\hat{x}(t')\rangle_{\mathcal{S}} \tag{6}$$

B – Equilibrium dynamics as a symmetry of MSR field theories

We first consider the case of equilibrium dynamics: (i) the force is assumed to be time-independent and to derive from the same potential as in the initial preparation: $f(x) = -\partial_x V(x)$; (ii) the bath temperature is assumed to be the same as in the initial preparation: $T = T_0$.

(1) Show that the functional $\mathcal{S}_{\text{bath}}[x, \hat{x}]$ in (4) is always invariant under the following transformation of the fields,

$$\mathcal{T}_\beta : \begin{cases} x(t) & \mapsto x(-t) \\ \mathrm{i}\hat{x}(t) & \mapsto \mathrm{i}\hat{x}(-t) + \beta \partial_t x(-t) \end{cases} . \tag{7}$$

(2) In equilibrium, show that the whole action functional $\mathcal{S}[x, \hat{x}]$ is symmetric under $\mathcal{T}_\beta$.

(3) Compute the Jacobian of the transformation $\mathcal{T}_\beta$.

(4) The path integrals in $\int \mathcal{D}[x, \hat{x}] \ldots \mathrm{e}^{-\mathcal{S}[x,\hat{x}]}$ are performed over real fields x and $\hat{x}$. Argue that, after the complex transformation $\mathcal{T}_\beta$ of $\hat{x}$, the integration domain of $\hat{x}(t)$ can be returned to real values. Conclude that, in thermal equilibrium, for any functional A of x and $\hat{x}$, we have the following Ward-Takahashi identities,

$$\langle A[x, \hat{x}] \rangle_{\mathcal{S}} = \langle A[\mathcal{T}_\beta x, \mathcal{T}_\beta \hat{x}] \rangle_{\mathcal{S}} . \tag{8}$$

(5) In particular, setting $A[x, \hat{x}] = x(t)x(t')$ and using the time-translational invariance of equilibrium dynamics, show the reciprocity relation $C(t - t') = C(t' - t)$.

(6) Fluctuation-dissipation theorem (FDT). Setting $A[x, \hat{x}] = x(t)\mathrm{i}\hat{x}(t')$, show the FDT

$$\begin{aligned} R(t - t') &= -\beta \, \partial_t C(t - t') \text{ for } t > t' , \\ &= 0 \text{ for } t \le t' . \end{aligned} \tag{9}$$

Discuss the profound implications of this theorem. Where are the fluctuations, where is the dissipation in Eq. (9)?

C – Non-equilibrium dynamics: symmetry breaking

We now consider the non-equilibrium situation in which the particle is subject to a *time-dependent* potential force: $f(x, t) = -\partial_x V(x, \lambda(t))$ where $\lambda(t)$ is an externally-controlled protocol (*e.g.* the push of a piston). Initially, the particle is prepared in thermal equilibrium at temperature $T_0 = T$ in the confining potential $V(x, \lambda(-t_0))$. The corresponding distribution function is $P(x, \dot{x}; -t_0) = \mathcal{Z}^{-1}(\lambda(-t_0)) \exp\left[-\beta\left(\frac{1}{2} m\dot{x}^2 + V(x, \lambda(-t_0))\right)\right]$.

(1) Show that the transformation of $\mathcal{S}[x, \hat{x}; \lambda]$ under the transformation $\mathcal{T}_\beta$ yields

$$\mathcal{S}[x, \hat{x}; \lambda] \mapsto \mathcal{S}[x, \hat{x}; \bar{\lambda}] + \beta \left(\mathcal{W}[x, \bar{\lambda}] - \Delta\mathcal{F}_{\text{r}}\right) \tag{10}$$

where $\bar{\lambda}(t) \equiv \lambda(-t)$ is the time-reversed protocol, $\Delta\mathcal{F}_{\text{r}} = -\ln \mathcal{Z}(\bar{\lambda}(t_0)) + \ln \mathcal{Z}(\bar{\lambda}(-t_0))$ is the change in free energy associated to this time-reversed protocol, and $\mathcal{W}[x, \bar{\lambda}]$ is the external work performed along a given trajectory $[x]$ under a protocol $\bar{\lambda}$.

(2) Recalling the first and second law of thermodynamics, argue that the quantity $\mathcal{W}[x, \lambda] - \Delta\mathcal{F}$ corresponds to the total amount of irreversible entropy $\mathcal{S}_{\text{irr}}[x; \lambda]$ generated by the protocol λ along a given trajectory $[x]$.

(3) Show that, for any functional A of x and $\hat{x}$, we have the identities

$$\mathrm{e}^{\beta\Delta\mathcal{F}}\langle A[x,\hat{x}]\mathrm{e}^{-\beta\mathcal{W}[x;\lambda]}\rangle_{\mathcal{S}[\lambda]} = \langle A[\mathcal{T}_\beta x,\mathcal{T}_\beta\hat{x}]\rangle_{\mathcal{S}[\bar{\lambda}]}\,. \tag{11}$$

(4) In particular, setting $A[x,\hat{x}]=1$, show the so-called Jarzynski equality,

$$\langle \mathrm{e}^{-\beta\mathcal{W}[x]}\rangle = \mathrm{e}^{-\beta\Delta\mathcal{F}}\,. \tag{12}$$

(5) Use Jensen's inequality, $\langle \mathrm{e}^{-X}\rangle \geq \mathrm{e}^{-\langle X\rangle}$, to show $\langle\mathcal{W}[x]\rangle \geq \Delta\mathcal{F}$. In which situations is the inequality an equality?

(6) Work fluctuation theorem. Setting $A[x,\hat{x}]=\delta(\mathcal{W}[x;\lambda]-\mathcal{W})$, show Crooks' fluctuation theorem

$$P_\lambda(\mathcal{W}) = P_{\bar{\lambda}}(-\mathcal{W})\,\mathrm{e}^{\beta(\mathcal{W}-\Delta\mathcal{F})}\,, \tag{13}$$

where $P_\lambda(\mathcal{W})$ is the probability to perform a total external work $\mathcal{W}$ with a given protocol λ.

(7) Fluctuation theorem (FT). Show and discuss the FT

$$P_\lambda(\mathcal{S}_{\mathrm{irr}}) = P_{\bar{\lambda}}(-\mathcal{S}_{\mathrm{irr}})\,\mathrm{e}^{\mathcal{S}_{\mathrm{irr}}}\,, \tag{14}$$

and show that the positivity of the irreversible entropy production is recovered *in average*, $\langle\mathcal{S}_{\mathrm{irr}}\rangle \geq 0$.

D – Challenge

Relax the assumption that the system is initially prepared in thermal equilibrium. The initial state is now simply characterized by the generic probability density $P(x,\dot{x};-t_0)$. Re-write the corresponding action functional, plug in the transformation $\mathcal{T}_\beta$, and generalize Jarzynski's equality (to the so-called Kawasaki's identity) and Crooks' fluctuation theorem.