Correlations in classical non-equilibrium systems and their connection with temperature

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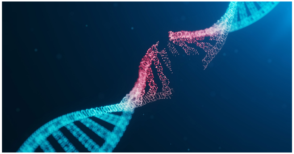
P²mc

Plasma **P**hysics, **M**atter and **C**omplexity

Comisión Chilena de Energía Nuclear


Non-equilibrium thermodynamics:

Steady states (e.g. superstatistics), maximum caliber models

Complexity and information:

Information entropy, Bayesian inference

Computational Statistical Mechanics:

Monte Carlo Simulation in generalized ensembles

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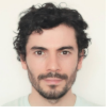

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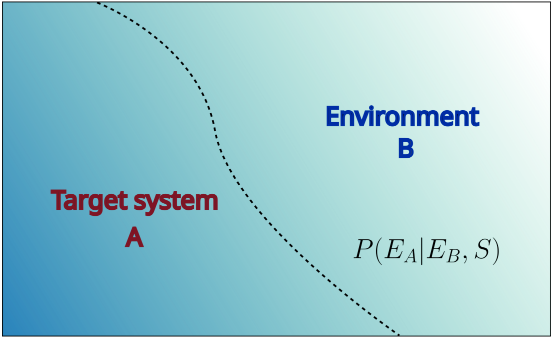
The main idea: correlation between subsystems

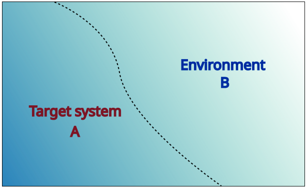


- Complex systems cannot be reduced to independent parts: correlations!
- Correlations are more important than interactions?
- What is temperature in non-equilibrium states?
- Connection between correlations and temperature fluctuations
- Invariant quantities upon the choice of target and environment

A composite system in canonical equilibrium

Neglecting the interaction energy, we have

$$\mathcal{H}_{AB}(\mathbf{\Gamma}_A, \mathbf{\Gamma}_B) = \mathcal{H}_A(\mathbf{\Gamma}_A) + \mathcal{H}_B(\mathbf{\Gamma}_B) + \cancelto{\approx 0}{\mathcal{H}_{\text{int}}(\mathbf{\Gamma}_A, \mathbf{\Gamma}_B)}$$



$$\begin{aligned}
P(\mathbf{\Gamma}_A, \mathbf{\Gamma}_B|\beta) &= \frac{\exp\big(-\beta\mathcal{H}_{AB}(\mathbf{\Gamma}_A, \mathbf{\Gamma}_B)\big)}{Z_{AB}(\beta)} \\
&= \frac{\exp\big(-\beta\mathcal{H}_A(\mathbf{\Gamma}_A)\big)}{Z_A(\beta)}\,\frac{\exp\big(-\beta\mathcal{H}_B(\mathbf{\Gamma}_B)\big)}{Z_B(\beta)} \\
&= P(\mathbf{\Gamma}_A|\beta)\,P(\mathbf{\Gamma}_B|\beta)
\end{aligned}$$

Canonical $\Longrightarrow$ uncorrelated therefore correlated $\Longrightarrow$ non-canonical

Correlations between target and environment imply non-canonical ensembles: **temperature fluctuations**

Steady-state ensembles out of equilibrium

$$P(\mathbf{\Gamma}|\beta) = \frac{\exp\big(-\beta\mathcal{H}(\mathbf{\Gamma})\big)}{Z(\beta)}$$

canonical ensemble

$$P(\mathbf{\Gamma}|E) = \frac{\delta\big(E-\mathcal{H}(\mathbf{\Gamma})\big)}{\Omega(E)}$$

microcanonical ensemble

We will generalize these cases to a **steady-state ensemble** of the form

$$\boxed{P(\mathbf{\Gamma}|S) = \rho\big(\mathcal{H}(\mathbf{\Gamma});S\big)}$$

where $\rho(\bullet;S)$ is the *ensemble function* with parameters S.

In general, the subsystems are not statistically independent,

$$P(\mathbf{\Gamma}_A,\mathbf{\Gamma}_B|S) = \rho\big(\mathcal{H}_A(\mathbf{\Gamma}_A)+\mathcal{H}_B(\mathbf{\Gamma}_B);S\big) \neq P(\mathbf{\Gamma}_A|S)\,P(\mathbf{\Gamma}_B|S). \tag{1}$$

- The ensemble can introduce **correlations even without interactions**
- These correlations may even be **long-ranged** (e.g. fixed global property)

Composite systems in general steady states

The distribution of the target is obtained by “integrating out” the environment,

$$P(\mathbf{\Gamma}_A|S) = \int d\mathbf{\Gamma}_B\, P(\mathbf{\Gamma}_A, \mathbf{\Gamma}_B|S) = \int d\mathbf{\Gamma}_B\, \rho\big(\mathcal{H}_A(\mathbf{\Gamma}_A) + \mathcal{H}_B(\mathbf{\Gamma}_B); S\big) = \rho_A\big(\mathcal{H}_A(\mathbf{\Gamma}_A); S\big)$$

It is a steady state but, in general, different in shape from the original:

$$\rho_A(E_A; S) = \int dE_B\, \Omega_B(E_B)\rho\big(E_A + E_B; S\big)$$

The ensemble function ρ_A for the target **will depend on the details** of the environment through its density of states.

The distribution of E_A and joint distribution of (E_A, E_B) are given by

$$P(E_A|S) = \Big\langle \delta\big(E_A - \mathcal{H}_A\big) \Big\rangle_S = \rho_A(E_A; S)\Omega_A(E_A)$$

$$P(E_A, E_B|S) = \Big\langle \delta\big(E_A - \mathcal{H}_A\big)\delta\big(E_B - \mathcal{H}_B\big) \Big\rangle_S = \rho(E_A + E_B; S)\Omega_A(E_A)\Omega_B(E_B)$$

The microcanonical inverse temperature

For an isolated composite system we have

$$\rho_A(E_A;E) = \int dE_B\,\Omega_B(E_B)\left[\frac{\delta\big(E-E_A-E_B\big)}{\Omega(E)}\right] = \frac{\Omega_B\big(E-E_A\big)}{\Omega(E)}$$

If the environment is large, that is, $E_A \ll E$, we can approximate

$$\ln\Omega_B(E-E_A) \approx \ln\Omega_B(E) - \partial_E \ln\Omega_B(E) E_A$$

$$\implies \rho_A(E_A|E) = \frac{\Omega_B\big(E-E_A\big)}{\Omega(E)} \approx \frac{\Omega_B(E)}{\Omega(E)}\exp\big(-\beta_E E_A\big)$$

$$\boxed{\beta_\Omega(E) := \frac{\partial}{\partial E}\ln\Omega(E)}$$

(microcanonical inverse temperature)

$$\beta_\Omega(E) = \frac{1}{k_B T} \text{ if } \frac{1}{T} = \frac{\partial \mathcal{S}(E)}{\partial E} \text{ and } \mathcal{S}(E) = k_B \ln\Omega(E)$$

This is an **intrinsic observable**: $\Omega(\bullet)$ only depends on the shape of $\mathcal{H}$

The fundamental inverse temperature

On the other hand, for any ensemble $P(\mathbf{\Gamma}|S) = \rho\big(\mathcal{H}(\mathbf{\Gamma}); S\big)$ we can define*

$$\boxed{\beta_F(E; S) := -\frac{\partial}{\partial E}\ln \rho(E; S)}$$

(fundamental inverse temperature)

This observable is **not intrinsic**: depends on the shape of the ensemble

$$\rho(E; \beta_0) = \frac{\exp(-\beta_0 E)}{Z(\beta_0)} \iff \beta_F(E; \beta_0) = \beta_0$$

- Canonical ensemble is equivalent to constant β_F
- Any ensemble other than canonical will have **temperature fluctuations**

$$\rho(E; A, E_0) = \frac{\exp\big(-A(E-E_0)^2\big)}{\eta_A(E_0)} \iff \beta_F(E; A, E_0) = 2A(E-E_0)$$

$$\rho(E; q, \beta_0) = \frac{1}{Z_q(\beta_0)}\Big[1+(q-1)\beta_0 E\Big]_+^{\frac{1}{1-q}} \iff \beta_F(E; q, \beta_0) = \frac{\beta_0}{1+(q-1)\beta_0 E}$$

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*S. Davis and G. Gutiérrez, Phys. A **533**, 122031 (2019).

Equivalence of temperatures in steady states

Fundamental and microcanonical temperatures have the same expectation,

$$\boxed{\beta_S := \big\langle \beta_F \big\rangle_S = \big\langle \beta_\Omega \big\rangle_S}$$

so it makes sense to take β_S as **the value** of the inverse temperature in S.

Naturally, β_S will agree with standard thermodynamics for the canonical and microcanonical ensembles.

Proof: The **conjugate variables theorem*** for the energy distribution

$$P(E|S) = \rho(E;S)\Omega(E)$$

is the following identity

$$\left\langle \frac{\partial \omega}{\partial E} \right\rangle_S = -\left\langle \omega \frac{\partial}{\partial E} \ln P(E|S) \right\rangle_S = \left\langle \omega \Big[\beta_F - \beta_\Omega \Big] \right\rangle_S \qquad (2)$$

valid for any differentiable $\omega(E)$.

Using $\omega(E) = 1$ we see that $0 = \big\langle \beta_F \big\rangle_S - \big\langle \beta_\Omega \big\rangle_S$ ■

*S. Davis, G. Gutiérrez. Phys. Rev. E **86**, 051136 (2012).

Marginalization property of the inverse temperature

Now recall the marginalization procedure to obtain ρ_A from ρ:

$$\rho_A(E_A; S) = \int dE_B\, \Omega_B(E_B)\rho(E_A + E_B; S) \tag{3}$$

If we define the fundamental inverse temperature of the target as

$$b_F(E_A; S) := -\frac{\partial}{\partial E_A} \ln \rho_A(E_A; S) \tag{4}$$

then one goes from β_F to b_F simply by taking expectation given E_A:

$$\boxed{b_F(E_A; S) = \big\langle \beta_F \big\rangle_{E_A, S}}$$

We will call this the **marginalization property** of β_F.

Remark: A canonical composite system has $\beta_F(\bullet; \beta_0) = \beta_0$ so we have

$$b_F(E_A; \beta_0) = \big\langle \beta_0 \big\rangle_{E_A, \beta_0} = \beta_0$$

hence every subsystem of a canonical system must be canonical.

Proof of the marginalization property

$$\boxed{b_F(E_A;S) = \big\langle \beta_F \big\rangle_{E_A,S}} \qquad \text{(MP)}$$

The conditional distribution of E_B given E_A in S is

$$P(E_B|E_A,S) = \frac{P(E_A,E_B|S)}{P(E_A|S)} = \frac{\rho(E_A+E_B;S)\cancel{\Omega_A(E_A)}\Omega_B(E_B)}{\rho_A(E_A;S)\cancel{\Omega_A(E_A)}}$$

and from it we can construct its **fluctuation-dissipation theorem***,

$$\begin{aligned}\frac{\partial}{\partial E_A}\big\langle \omega \big\rangle_{E_A,S} &= \left\langle \frac{\partial \omega}{\partial E_A} \right\rangle_{E_A,S} + \left\langle \omega\,\frac{\partial}{\partial E_A}\ln P(E_B|E_A,S)\right\rangle_{E_A,S} \\ &= \left\langle \frac{\partial \omega}{\partial E_A} \right\rangle_{E_A,S} + \Big\langle \omega\Big[b_F - \beta_F\Big]\Big\rangle_{E_A,S}\end{aligned}$$

which is an identity for any function $\omega(E_A,E_B)$ differentiable on E_A.

Choosing $\omega(E_A,E_B) = 1$ we immediately prove our result, as we have

$$0 = \big\langle b_F - \beta_F \big\rangle_{E_A,S} = b_F(E_A;S) - \big\langle \beta_F \big\rangle_{E_A,S} \qquad \blacksquare$$

*S. Davis, G. Gutiérrez. AIP Conf. Proc. **1757**, 020002 (2016).

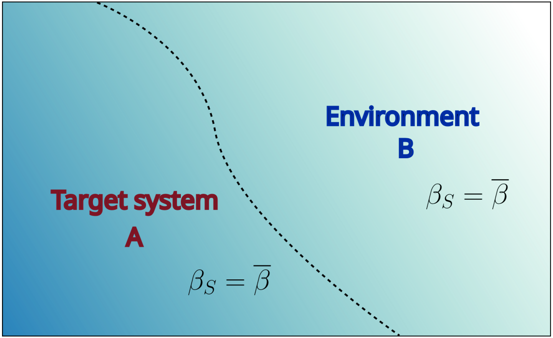
Steady-state ensembles have a kind of equilibrium?

$$\boxed{b_F(E_A; S) = \big\langle \beta_F \big\rangle_{E_A,S}} \qquad \text{(MP)}$$

Taking expectation under S on both sides of (MP) we see that

$$\big\langle b_F \big\rangle_S = \Big\langle \big\langle \beta_F \big\rangle_{E_A,S} \Big\rangle_S = \big\langle \beta_F \big\rangle_S = \beta_S. \tag{5}$$

In other words, β_S **is invariant** with respect to the choice of subsystem.



A new invariance in steady-state ensembles

Let us write the fluctuation-dissipation theorem for E_B given E_A under S,

$$\frac{\partial}{\partial E_A}\big\langle \omega \big\rangle_{E_A,S} = \Big\langle \frac{\partial \omega}{\partial E_A} \Big\rangle_{E_A,S} + \Big\langle \omega \Big[b_F - \beta_F\Big] \Big\rangle_{E_A,S}$$

and now use the choice $\omega(E_A, E_B) = \beta_F(E_A + E_B; S)$. We obtain

$$\begin{aligned}
\frac{\partial}{\partial E_A}\big\langle \beta_F \big\rangle_{E_A,S} = {b_F}'(E_A;S) = \big\langle {\beta_F}' \big\rangle_{E_A,S} + b_F(E_A;S)^2 - \big\langle {\beta_F}^2 \big\rangle_{E_A,S} \\
\hookrightarrow b_F(E_A;S)^2 - {b_F}'(E_A;S) = \big\langle {\beta_F}^2 \big\rangle_{E_A,S} - \big\langle {\beta_F}' \big\rangle_{E_A,S} \\
\hookrightarrow \big\langle {b_F}^2 \big\rangle_S - \big\langle {b_F}' \big\rangle_S = \big\langle {\beta_F}^2 \big\rangle_S - \big\langle {\beta_F}' \big\rangle_S
\end{aligned}$$

where in the last line we have taken $\big\langle \bullet \big\rangle_S$ on both sides.

Using $\beta_S = \big\langle \beta_F \big\rangle_S = \big\langle b_F \big\rangle_S$ and substracting $(\beta_S)^2$ from both sides we get

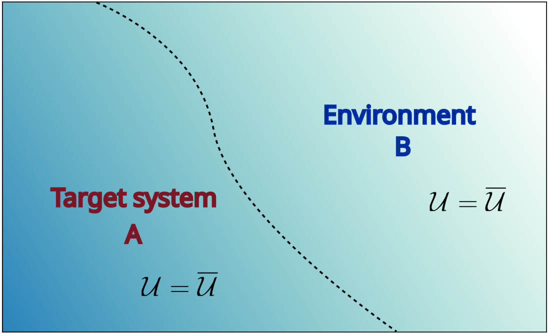
$$\big\langle (\delta b_F)^2 \big\rangle_S - \big\langle {b_F}' \big\rangle_S = \big\langle (\delta \beta_F)^2 \big\rangle_S - \big\langle {\beta_F}' \big\rangle_S \tag{6}$$

A new invariance in steady-state ensembles

Therefore we can define a new, invariant quantity*

$$\boxed{\mathcal{U} := \big\langle (\delta\beta_F)^2 \big\rangle_S - \big\langle {\beta_F}' \big\rangle_S}$$

(inverse temperature covariance)



$$\mathcal{U}_A = \mathcal{U}_B = \mathcal{U}_{AB}$$

As the canonical ensemble has constant β_F, we must have $\mathcal{U}_{\text{canon}} = 0$.

*S. Davis. Phys. A **608**, 128249 (2022).

The inverse temperature covariance

The conjugate variables theorem for $P(E|S)$,

$$\left\langle \frac{\partial \omega}{\partial E} \right\rangle_S = \left\langle \omega \Big[\beta_F - \beta_\Omega\Big] \right\rangle_S$$

reveals different expressions for $\mathcal{U} = \big\langle(\delta\beta_F)^2\big\rangle_S - \big\langle{\beta_F}'\big\rangle_S$.

$\omega(E) = \beta_F(E)$:

$$\big\langle {\beta_F}' \big\rangle_S = \big\langle {\beta_F}^2 \big\rangle_S - \big\langle \beta_F\beta_\Omega \big\rangle_S \qquad \text{therefore} \qquad \boxed{\mathcal{U} = \big\langle \delta\beta_F\delta\beta_\Omega \big\rangle_S}$$

$\omega(E) = \beta_\Omega(E)$:

$$\big\langle {\beta_\Omega}' \big\rangle_S = \big\langle \beta_\Omega\beta_F \big\rangle_S - \big\langle {\beta_\Omega}^2 \big\rangle_S \qquad \text{therefore} \quad \mathcal{U} = \big\langle(\delta\beta_\Omega)^2\big\rangle_S + \big\langle {\beta_\Omega}' \big\rangle_S$$

Both β_S and $\mathcal{U}$ can, in principle, be “measured” for a system if we know the density of states of one of its subsystems

The inverse temperature covariance

Another valid expression for $\mathcal{U}$ is $\boxed{\mathcal{U} = \big\langle \delta b_\Omega \delta \mathcal{B}_\Omega \big\rangle_S}$

This means $\mathcal{U} \neq 0$ signals **correlation between subsystems**

Proof: For the conditional distribution $P(E_B|E_A, S) = \dfrac{\rho(E_A + E_B; S)\Omega_B(E_B)}{\rho_A(E_A; S)}$ we construct its conjugate variables theorem,

$$\left\langle \frac{\partial \omega}{\partial E_B} \right\rangle_{E_A,S} = \Big\langle \omega \big[\beta_F - \mathcal{B}_\Omega\big] \Big\rangle_{E_A,S} \tag{7}$$

Using $\omega(E_A, E_B) = 1$ we have $0 = \cancelto{b_F}{\big\langle \beta_F \big\rangle_{E_A,S}} - \big\langle \mathcal{B}_\Omega \big\rangle_{E_A,S}$ and it follows that

$$
\begin{aligned}
& b_F(E_A; S) = \big\langle \mathcal{B}_\Omega \big\rangle_{E_A,S} \\
\hookrightarrow\ & b_F(E_A; S) b_\Omega(E_A; S) = \big\langle b_\Omega \mathcal{B}_\Omega \big\rangle_{E_A,S} \\
\hookrightarrow\ & \big\langle b_F b_\Omega \big\rangle_S - (\beta_S)^2 = \big\langle b_\Omega \mathcal{B}_\Omega \big\rangle_S - (\beta_S)^2 \quad \blacksquare
\end{aligned}
$$

Case study: Superstatistics (Beck & Cohen, 2003)

Superstatistics is a steady-state theory with β a "random variable" such that

$$P(\mathbf{\Gamma},\beta|S) = P(\beta|S)P(\mathbf{\Gamma}|\beta) = P(\beta|S)\frac{\exp\big(-\beta\mathcal{H}(\mathbf{\Gamma})\big)}{Z(\beta)}$$

$$\rho(E;S) = \int_0^\infty d\beta f(\beta)\exp(-\beta E) \quad \text{with} \quad f(\beta) := \frac{P(\beta|S)}{Z(\beta)}$$

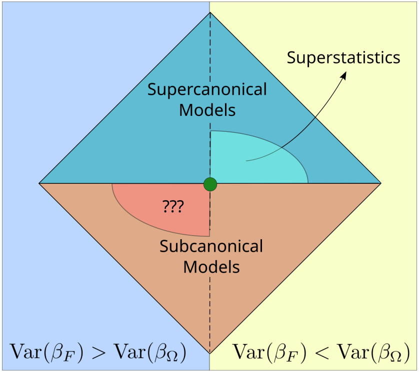
$$\beta_F(E;S) = \langle\beta\rangle_{E,S}$$

$$\boxed{\beta_S = \langle\beta\rangle_S}$$

$${\beta_F}'(E;S) = {\beta_F}^2(E;S) - \langle\beta^2\rangle_{E,S}$$

$$\boxed{\mathcal{U} = \langle(\delta\beta)^2\rangle_S \geq 0}$$

$$\mathcal{U} = 0 \iff \text{canonical}$$



S. Davis. Phys. A **589**, 126665 (2022).

Case study: Superstatistics (Beck & Cohen, 2003)

For a composite system, superstatistics looks like

$$\boxed{P(\mathbf{\Gamma}_A, \mathbf{\Gamma}_B|S) = \int_0^\infty d\beta\, P(\beta|S)P(\mathbf{\Gamma}_A, \mathbf{\Gamma}_B|\beta)}$$

$$P(\mathbf{\Gamma}_A|S) = \int d\mathbf{\Gamma}_B \int_0^\infty d\beta\, P(\beta|S)P(\mathbf{\Gamma}_A, \mathbf{\Gamma}_B|\beta) = \int_0^\infty d\beta\, P(\beta|S) \underbrace{\int d\mathbf{\Gamma}_B P(\mathbf{\Gamma}_A, \mathbf{\Gamma}_B|\beta)}_{=P(\mathbf{\Gamma}_A|\beta)}$$

The target distribution involves the same $P(\beta|S)$ as the composite system,

$$\boxed{P(\mathbf{\Gamma}_A|S) = \int_0^\infty d\beta\, P(\beta|S)P(\mathbf{\Gamma}_A|\beta)}$$

In superstatistics, the whole distribution $P(\beta|S)$ is invariant upon the choice of subsystem, so clearly β_S and $\mathcal{U}$ (its mean and variance) are.

Thank you!

As a summary:

- Steady-state ensembles have a well-defined temperature: $\beta_F(E; S)$
- For a subsystem, b_F is directly related to β_F of the entire system
- There are (at least) two invariant quantities in steady-state ensembles:

$$\beta_S := \big\langle \beta_F \big\rangle_S$$
$$\mathcal{U} := \big\langle (\delta\beta_F)^2 \big\rangle_S - \big\langle {\beta_F}' \big\rangle_S$$

- Correlations between subsystems are related to $\mathcal{U}$ (fluctuations of β_F)
- Superstatistics fits nicely, but there is a whole space of models outside it

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