Stochastic systems with mixed boundary conditions in time

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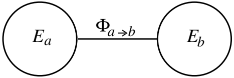
Stochastic atom model

- I want to generate an arrow of time from a microscopic reversible dynamics. The ultimate aim is to study the interaction of systems with conflicting arrows of time,
- Deterministic chaos: too difficult for me.
- Langevin dynamics already dissipative.
- Stochastic atom model from analogy with radiation theory $w_{N \to N-1} = |\langle N-1|c|N\rangle|^2 = |\langle N|c^+|N-1\rangle|^2 = w_{N-1 \to N} \Rightarrow$



$$w(E_a, E_b \to E_a + \Delta E, E_b + \Delta E) =$$
$$= w(E_a + \Delta E, E_b - \Delta E \to E_a, E_b) = \Gamma(E_a + \Delta E) E_b$$

- Energy conservation; $E_{a,b}$ positive defined.

Strong detailed balance

- Microscopic reversibility implies uniform equilibrium distribution:

$$w(\mathbf{E}'; t'|\mathbf{E}, t) = w(\mathbf{E}; t'|\mathbf{E}', t) \Rightarrow \bar{P}(\mathbf{E}') = \bar{P}(\mathbf{E})$$

Extension to the case of N atoms

- Microcanonical equilibrium distribution.
- We can prove the law of increase for the entropy $S(t) = -\langle \ln P(\mathbf{E}, t) \rangle$, $\dot{S} \geq 0$.

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SDE representation

- Continuous limit $\Delta E \to 0$

$$\mathrm{d}E_a = \Gamma(E_b - E_a)\mathrm{d}t + \sqrt{2\Gamma E_a E_b}\,\mathrm{d}W, \quad \langle \mathrm{d}W^2\rangle = \mathrm{d}t;$$
$$\partial_t P = \Gamma \partial_{E_a}(E_a E_b \partial_{E_a} P).$$

Interaction with a thermal bath

- Atom a becomes *the system*. Many atoms b together form *the thermostat*.

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- The associated Fokker-Planck equation reads

$$\partial_t P = \Gamma \partial_{E_a}[E_a(P + T\partial_{E_a} P)].$$

- At equilibrium we get the Boltzmann distribution

$$\bar{P}(E_a) = (1/T)\exp(-E_a/T). \tag{1}$$

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- If the system contains $N \gg 1$ atoms, we get the Langevin equation

$$\mathrm{d}\tilde{E}_a = -\Gamma\tilde{E}_a\mathrm{d}t + \sqrt{2\Gamma N}T\,\mathrm{d}W, \qquad \tilde{E}_a = E_a - NT. \tag{2}$$

Additional properties

- It is possible to prove that $P(E,t)$ approaches equilibrium by first relaxing onto a time-dependent Boltzmann distribution:

$$P(E_a,t) \longrightarrow \frac{1}{\langle E_a(t)\rangle} \exp\Big(-\frac{E_a}{\langle E_a(t)\rangle}\Big) \longrightarrow \frac{1}{T} \exp\Big(-\frac{E_a}{T}\Big).$$

- If the relaxation of the thermal bath is faster than that of the system, the total entropy $S = S_a + S_{bath}$ of the system + thermostat obeys

$$\dot{S} = \dot{S}_a - \frac{\langle \dot{E}_a \rangle}{T} \geq 0.$$

Few remarks on time arrows and reversibility

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- After averaging, the drift becomes *de facto* a dissipation (a thermodynamic limit is actually required, but this is more a matter of interpretation).
- Microscopic reversibility is replaced by macroscopic reversibility, i.e. by standard detailed balance

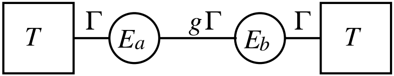
$$P(\mathbf{E}', t'|\mathbf{E}, t)\bar{P}(\mathbf{E}) = P(\mathbf{E}, t'|\mathbf{E}', t)\bar{P}(\mathbf{E}').$$

- Detailed balance implies the reversibility relation

$$P(\mathbf{E}', t'|\mathbf{E}, t) = P(\mathbf{E}', t|\mathbf{E}, t'). \tag{3}$$

- This tells us that the time reversed dynamics conditioned in the future is identical to the original dynamics conditioned in the past. The choice of conditioning determines the arrow of time for the system.

Two atoms in a thermal bath



- Forward dynamics quite easy to study:
  - Initial conditions $\mathbf{E}(t_i) = \mathbf{E}^i$.
  - We can write SDE and Fokker-Planck equations to describe the heat transfer
  - Boltzmann equilibrium

$$\bar{P}(\mathbf{E}) = T^{-2} \exp[-(E_a + E_b)/T].$$

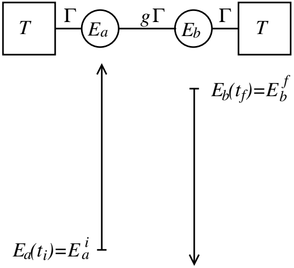
  - Mean heat transfer

$$\langle \dot{E}_a \rangle = \Gamma[T - \langle E_a \rangle + g\langle E_b - E_a \rangle]; \ \langle \dot{E}_b \rangle = \Gamma[T - \langle E_b \rangle - g\langle E_b - E_a \rangle].$$

  - Total entropy growth

$$\dot{S} = \frac{\Gamma}{T^2}[(\langle E_a \rangle - T)^2 + (\langle E_b \rangle - T)^2 + g(\langle E_a \rangle - \langle E_b \rangle)^2] \geq 0.$$

- Impose boundary condition in the past on a and in the future on b.



Incomplete Schrödinger bridge

$$
\begin{aligned}
&P(\mathbf{E}, t|E_a^i, t_i; E_b^f, t_f) \\
&= \frac{P(E_b^f, t_f|\mathbf{E}, t; E_a^i, t_i)P(\mathbf{E}, t; E_a^i, t_i)}{\bar{P}(E_a^i, t_i; E_b^f, t_f)} \\
&= \frac{P(E_b^f, t_f|\mathbf{E}, t)P(\mathbf{E}, t|E_a^i, t_i)}{P(E_b^f, t_f|E_a^i, t_i)}.
\end{aligned}
$$

- Boundary conditions:

$$
\begin{aligned}
P(\mathbf{E}, t_i|E_a^i, t_i) &= \delta(E_a - E_a^i)\bar{P}(E_b) \\
P(E_b, t_f|\mathbf{E}^f, t_f) &= \delta(E_b - E_b^f).
\end{aligned}
$$

Opposite arrows of time

- Alternative form of Schrödinger bridge formula

$$P(\mathbf{E}, t|E_a^i, t_i; E_b^f, t_f) = \frac{P(\mathbf{E}, t|E_a^i, t_i)}{\bar{P}(E_b)} \, \frac{P(\mathbf{E}, t|E_b^f, t_f)}{\bar{P}(E_a)} \, \frac{\bar{P}(E_a^i)\bar{P}(E_b^f)}{\bar{P}(E_a^i, t_i; E_b^f, t_f)}.$$

- The approach to equilibrium in opposite directions of time becomes evident when a and b are decoupled:
  $P(\mathbf{E}, t|E_a^i, t_i)/\bar{P}(E_b) = P(E_a, t|E_a^i, t_i)$;
  $P(\mathbf{E}, t|E_b^f, t_f)/\bar{P}(E_a) = P(E_b, t|E_b^f, t_f)$.
- Note the complete symmetry of the Schrödinger bridge expression with respect to boundary conditions in the past and in the future.

Conflicting relaxation

- Far from the boundaries, $P(\mathbf{E}, t)$ is instantaneously Boltzmann.
- Its evolution can be described in terms of the temperature anomaly $\hat{E}_{a,b} \equiv E_{a,b}/T - 1$:

$$
\begin{aligned}
\langle \hat{E}_a(t) | E_a^i, t_i; E_b^f, t_f \rangle &= A(t - t_i)\hat{E}_a^i + B(t_f - t)\hat{E}_b^f, \\
\langle \hat{E}_b(t) | E_a^i, t_i; E_b^f, t_f \rangle &= B(t - t_i)\hat{E}_a^i + A(t_f - t)\hat{E}_b^f,
\end{aligned}
$$

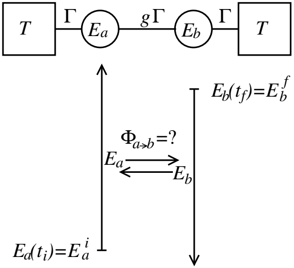
  where $A(0) = 1$, $B(0) = 0$, $A(t) = B(t) \to 0$ for $t \to +\infty$.
- For the entropy,

$$
\dot{S} = A(t - t_i)(\hat{E}_a^i)^2 - A(t_f - t)(\hat{E}_b^f)^2. \tag{4}
$$

- No contribution to entropy dynamics from the mutual interaction of the atoms.

Heat fluxes

- It is not clear if heat should flow from a to b or vice versa.



Calculation in large deviation regime

- Heat flux dominated by the noise component in the SDE, that steers $E_b(t)$ towards E_b^f.

$$\begin{aligned}\Phi_{a\to b} &= g\Gamma[\hat{E}_a^i \mathrm{e}^{-(1+2g)\Gamma(t-t_i)} \\ &+ \hat{E}_b^f \mathrm{e}^{-(1+2g)\Gamma(t_f-t)}].\end{aligned}$$

- No contribution to $\Phi_{a\to b}$ from $E_a - E_b$.

Summarizing:

- Near the boundaries, the dynamics is dominated by relaxation of the conditioned systems towards equilibrium: system a in the future; system b in the past.
- For large $t_f - t_i$, near t_i, b is enslaved to a; near t_f, a is enslaved to b.
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- The answer is yes (see e.g. Ma and Yong, Springer 2007), but we lose the symmetric description of boundary conditions afforded by the Schrödinger bridge approach.
- What is the physical meaning of the choice of time direction implicit in a SDE approach?

Small philosophical aside

- We can see a stochastic process as a tool to generate trajectories distributed with a given statistics.
- Different stochastic processes can generate the same trajectory statistics. In particular, we can generate a given statistics both from stochastic processes that evolve forward, and from stochastic processes that evolve backward in time.
- A causal response can be defined as a response that does not require sampling in order to be detected in a (forward) experiment. Obviously, a causal response is more naturally described in a forward picture.
- A causal response and a forward description are more natural both from the point of experiment and of theoretical picture if the system is conditioned in the past. Things are less clear if the system is conditioned in the future.

The problem from the point of view of experiments

- Suppose that the system is perturbed at time $t = 0$ by a Dirac delta forcing. Identify with tilde perturbed quantities. The system has boundary condition $x(t_f) = x_f,\ t_f > 0$.
- Response of the system to external perturbation more easily detected by first perturbing the system and then sampling trajectories. Not vice versa.
- Schrödinger bridge representation:

$$\tilde{P}(x, t < 0|x_f, t_f) = \frac{\tilde{P}(x_f, t_f|x, t)\tilde{P}(x, t < 0)}{\tilde{P}(x_f, t_f)} = \frac{\tilde{P}(x_f, t_f|x, t)\bar{P}(x)}{\tilde{P}(x_f, t_f)},$$

$$\tilde{P}(x, t > 0|x_f, t_f) = \frac{\tilde{P}(x_f, t_f|x, t > 0)\tilde{P}(x, t)}{\tilde{P}(x_f, t_f)} = \frac{P(x_f, t_f|x, t)\tilde{P}(x, t)}{\tilde{P}(x_f, t_f)}.$$

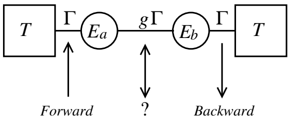
- The probability receives an anticipating correction from the perturbation through the factor $\tilde{P}(x_f, t_f|x, t)\bar{P}(x)/\tilde{P}(x_f, t_f)$.

The problem from the point of view of theory

- We have seen that, in the presence of conditioning in the future, the kind of response that is experimentally easier to detect, has some non-causal features.
- From the point of view of theory, a simpler physical picture is obtained by means of a fully backward description and a fully anticausal response.
- We wonder what would be the most natural description (at least from the point of theory) in the case of a system with mixed boundary conditions in time.

Possibility of a mixed forward-backward description

- Main motivation:
  - If a and b are decoupled, the most natural description of the dynamics is forward in time for a and backward in time for b.
  - We wonder whether the description could be adapted, with some sort of perturbation expansion around the uncoupled case, to the case a and b are weakly coupled.
- Main difficulty:
  - A stochastic process cannot simultaneously evolve (be "adapted") forward and backward in time.
  - The interaction of a and b seem to require precisely such property:



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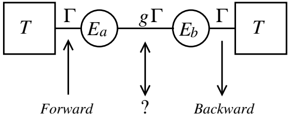

- Possible solution: to treat the interaction alternatively forward and backward in time in the perturbation expansion, depending on the need.

Application: Response to a delta function forcing

- We have the system of equation for the moments of $\mathbf{E}(t)$, after normalizing t and $\mathbf{E}$ in appropriate way and subtracting equilibrium values:

$$\begin{aligned} \langle \dot{E}_a(t) \rangle &= -\langle E_a(t) \rangle + g[\langle E_b(t) \rangle - \langle E_a(t) \rangle]; \\ \langle \dot{E}_b(t) \rangle &= \langle E_b(t) \rangle + g[\langle E_b(t) \rangle - \langle \tilde{E}_a(t) \rangle]. \end{aligned}$$

- Force E_a at time $t = 0$ with a Dirac delta of amplitude ξ and perturbatively evaluate the response, $\langle \mathbf{E} \rangle = \sum \langle \mathbf{E} \rangle^{(n)} g^n$. At $O(g^0)$ we solve for $\langle E_a \rangle$ forward in time to get

$$\langle E_a(t) \rangle^{(0)} = \xi \theta(t) \exp(-t)$$

- At the next two orders, solve for $\langle E_b \rangle$ and $\langle E_a \rangle$ backward and forward in time, respectively:

$$\begin{aligned} \langle E_b(t) \rangle^{(1)} &= (\xi/2) \exp(-|t|); \\ \langle E_a(t) \rangle^{(2)} &= (\xi/4)[1 + (2 + t) t \theta(t)] \exp(-|t|). \end{aligned}$$

- The backward response of E_b induces an anticipatory response for a.

Timemachine paradox

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- A timemachine "paradox" is generated if the anticipatory response is observed, but the perturbation is not enacted.
- Of course no paradox is generated in the stochastic case: the system is simply pushed on a less probable trajectory.
- We can define a probability cost of "solving the paradox" as the probability that the system response is generated without perturbation.
- This quantity can be calculated in the case a and b are each composed of $N \gg 1$ atoms, in such a way to work in a large deviation regime. In this case the probability cost is just the equilibrium probability of observing the value of the anticipatory response at $t = 0$:

$$P_{cost} \sim \exp\left(-\frac{Ng^4\xi^2}{32}\right).$$

Application: temperature shift

- Changing the temperature influences the noise part of the dynamics. The mixed forward-backward response generates nonlinear feedback on the drift. Suppose we increase linearly the temperature of thermostat a from T to $T+\delta T$ in the interval $[0,\delta t]$. The perturbation on E_a at time $t=\delta t$ is

$$\Delta E_a = \frac{\delta T}{2}\sqrt{\frac{E_a(0)}{2}}\Delta W_{at}(0).$$

- We can calculate again the $O(g^2)$ component of the perturbation to E_a at time $t=0$,

$$\langle E_a(0)\rangle^{(2)} = \frac{g^2}{4}\delta T\sqrt{2E_a(0)}\Delta W_{at}(0),$$

- ΔE_a contains through $E_a(0)$ the anticipary component of the perturbation. We have therefore to take into account a Zakai-Wong kind of correction, which leads to a rectifying effect on the response:

$$\langle \dot{E}_a\rangle \simeq \frac{g^2\,\dot{T}}{4}.$$

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- Possible experimental tests.