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BA Notes

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Contents

1 Theorems

1.1 Equipartition Theorem

Define the canonical position $\mathbf{q}$ and momentum $\mathbf{p}$ which follow Hamilton's equations

$$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \frac{\partial H}{\partial \mathbf{p}}, \tag{1}$$
$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\frac{\partial H}{\partial \mathbf{q}}. \tag{2}$$

where $H(\mathbf{p}, \mathbf{q})$ is the Hamiltonian.

In the canonical ensemble, consider a system in thermal equilibrium with an infinite heat bath at temperature T. The probability of each state in phase space is given by its Boltzmann factor times a normalization factor C, which is chosen so that the probabilities sum to one:

$$C \int e^{-\beta H(\mathbf{p},\mathbf{q})} d\Gamma = 1 \tag{3}$$

with the inverse temperature $\beta = 1/(k_\mathrm{B}T)$ and the infinitesimal volume

$$d\Gamma = \prod_i dp_i dq_i. \tag{4}$$

Using the product rule, we can derive the formula for integration by parts for a phase space variable x_k and an arbitrary function $f(\mathbf{p}, \mathbf{q})$

$$\int_a^b \frac{\mathrm{d}x_k f(\mathbf{p},\mathbf{q})}{\mathrm{d}x_k} dx_k = \int_a^b x_k f(\mathbf{p},\mathbf{q}) dx_k + \int_a^b x_k \frac{\mathrm{d}f(\mathbf{p},\mathbf{q})}{\mathrm{d}x_k} dx_k. \tag{5}$$

Using partial integration on Equation 3, we obtain

$$\begin{aligned} C \int \frac{\mathrm{d}x_k e^{-\beta H(\mathbf{p},\mathbf{q})}}{\mathrm{d}x_k} d\Gamma &= C \int x_k e^{-\beta H(\mathbf{p},\mathbf{q})} d\Gamma_k \\ &= C \int e^{-\beta H(\mathbf{p},\mathbf{q})} d\Gamma + C \int x_k \frac{\mathrm{d}e^{-\beta H(\mathbf{p},\mathbf{q})}}{\mathrm{d}x_k} d\Gamma \end{aligned} \tag{6}$$

where $d\Gamma_k = d\Gamma/dx_k$. Since $H(\mathbf{p}, \mathbf{q})$ describes a physical system, its Hamiltonian has to go to infinity as its canonical position and momentum go to infinity.
Also, since p_k and q_j are canonically assumed to be independent variables, the total derivative d/d_k simplifies to the partial derivative $\partial/\partial x_k$. Applying these two assumptions and using the chain rule on the last term allows a simplification of the expression above:

$$\begin{aligned} C \int x_k e^{-\beta H(\mathbf{p},\mathbf{q})} d\Gamma_k = 0 &= C \int e^{-\beta H(\mathbf{p},\mathbf{q})} d\Gamma + C \int x_k \frac{\mathrm{d}e^{-\beta H(\mathbf{p},\mathbf{q})}}{\mathrm{d}x_k} d\Gamma \\ &= 1 - C \int \beta x_k \frac{\partial H(\mathbf{p},\mathbf{q})}{\partial x_k} e^{-\beta H(\mathbf{p},\mathbf{q})} x_k d\Gamma \end{aligned} \tag{7}$$

Rearranging yields

$$C \int x_k \frac{\partial H(\mathbf{p},\mathbf{q})}{\partial x_k} e^{-\beta H(\mathbf{p},\mathbf{q})} x_k d\Gamma = \left\langle x_k \frac{\partial H(\mathbf{p},\mathbf{q})}{\partial x_k} \right\rangle = \frac{1}{\beta} = k_\mathrm{B} T \tag{8}$$

This result is called the Equipartition theorem. Assumptions:

1. Classical (Boltzmann statistics)

2. Thermal equilibrium with an infinite heat bath at temperature T

1.2 Interchanging Expectation and Derivative

1.2.1 Ansatz: Leibnitz Rule

Suppose

$$F(t) = \int_\Omega f(x,t)dx \tag{9}$$

We want to evaluate:

$$\frac{dF}{dt} = \frac{d}{dt}\int_\Omega f(x,t)\,dx = \int_\Omega \frac{\partial f(x,t)}{\partial t}dx \tag{10}$$

This interchange is valid under the conditions

1. Continuity of the Partial Derivative : $\frac{\partial f(x,t)}{\partial t}$ exists and is continuous with respect to both x and t.

2. Dominated Convergence: There exists an integrable function $g(x)$, independent of t, such that: $\left|\frac{\partial f(x,t)}{\partial t}\right| \leq g(x)$ for all $x \in \Omega$

This result can be extended to a multivariate function $f(\mathbf{x}, t)$ via Riemann integrals.

Now, let $f(x,t) = p(x,t)g(x,t)$, where $p(x,t)$ is a Probability Density Function (PDF) and $g(x,t)$ is an arbitrary function. Let all of the assumptions above apply. Then,

$$F(t) = \int_\Omega p(x,t)g(x,t)dx = \langle g(x,t)\rangle \tag{11}$$

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \frac{\mathrm{d}\,\langle g(x,t)\rangle}{\mathrm{d}t} = \int_\Omega g(x,t)\frac{\partial p(x,t)}{\partial t}dx + \int_\Omega p(x,t)\frac{\partial g(x,t)}{\partial t}dx \tag{12}$$

The expression above can be expressed in terms of expected values by using

$$\frac{\partial p(x,t)}{\partial t} = p(x,t)\frac{\partial \ln(p(x,t))}{\partial t}. \tag{13}$$

Substituting yields

$$\frac{\mathrm{d}\,\langle g(x,t)\rangle}{\mathrm{d}t} = \int_\Omega g(x,t)p(x,t)\frac{\partial \ln(p(x,t))}{\partial t}dx + \int_\Omega p(x,t)\frac{\partial g(x,t)}{\partial t}dx \tag{14}$$

$$= \left\langle \frac{\partial g(x,t)}{\partial t}\right\rangle + \left\langle g(x,t)\frac{\partial \ln(p(x,t))}{\partial t}\right\rangle \tag{15}$$

If the PDF does not depend on t, the expression simplifies to

$$\frac{\mathrm{d}\,\langle g(x,t)\rangle}{\mathrm{d}t} = \left\langle \frac{\partial g(x,t)}{\partial t}\right\rangle \tag{16}$$

1.2.2 Ansatz: Difference Quotient

Let $\left|\frac{\partial}{\partial t} g(\tau(h), x)\right| \leq Z$.

$$\frac{\partial}{\partial t}\mathbb{E}\big[g(t,x)\big] = \lim_{h\to 0}\frac{1}{h}\Big(\mathbb{E}\big[g(t+h,x)\big] - \mathbb{E}\big[g(t,x)\big]\Big) \tag{17}$$

$$= \lim_{h\to 0}\mathbb{E}\left[\frac{g(t+h,x)-g(t,x)}{h}\right] \tag{18}$$

$$= \lim_{h\to 0}\mathbb{E}\left[\frac{\partial}{\partial t} g(\tau(h),x)\right] \tag{19}$$

where $\tau(h) \in (t, t+h)$ exists by the Mean Value Theorem. By assumption we have

$$\left|\frac{\partial}{\partial t} g(\tau(h), x)\right| \leq Z \tag{20}$$

and thus we can use the Dominated Convergence Theorem to conclude

$$\frac{\partial}{\partial t}\mathbb{E}\big[g(t,x)\big] = \mathbb{E}\left[\lim_{h\to 0}\frac{\partial}{\partial t} g(\tau(h),x)\right] = \mathbb{E}\left[\frac{\partial}{\partial t} g(t,x)\right]. \tag{21}$$

1.3 Probability Current

A general probability current is defined as

$$\mathbf{J}(\mathbf{x}) = p(\mathbf{x})P(\mathbf{x}' \mid \mathbf{x}) - (\mathbf{x}')P(\mathbf{x} \mid \mathbf{x}') \tag{22}$$

where $P(\mathbf{x}' \mid \mathbf{x})$ is the transition PDF of the transition from a state $\mathbf{x} \to \mathbf{x}'$ and $P(\mathbf{x} \mid \mathbf{x}')$ is the probability of its reverse $\mathbf{x}' \to \mathbf{x}$. In equilibrium, the probability current vanishes. This is called detailed balance.

1.4 Wiener Processes

The Wiener Process is a continuous-time stochastic process $\{W(t)\}_{t\geq 0}$ characterized by:

1. Initial condition:
$$W(0) = 0 \quad \text{(almost surely)} \tag{23}$$

2. Independent increments: For any $0 \leq t_1 < t_2 < \cdots < t_n$,
$$W(t_{k+1}) - W(t_k) \text{ are independent random variables} \tag{24}$$

3. Gaussian increments:
$$W(t) - W(s) \sim \mathcal{N}(0, t-s) \quad \text{for } t > s \geq 0 \tag{25}$$

4. Continuous paths:
$$t \mapsto W(t) \text{ is almost surely continuous} \tag{26}$$

1.5 Ito SDE

An Ito Stochastic Differential Equation describes a process $\mathbf{X}(t) \in \mathbb{R}^n$ subject to random noise:

$$d\mathbf{x}(t) = \mathbf{A}(\mathbf{x}, t)\, dt + \mathbf{B}(\mathbf{x}, t)\, d\mathbf{W}(t) \tag{27}$$

where:

- $\mathbf{A} : \mathbb{R}^n \times [0, \infty) \to \mathbb{R}^n$ is the drift (deterministic component)
- $\mathbf{B} : \mathbb{R}^n \times [0, \infty) \to \mathbb{R}^{n\times m}$ is the diffusion (noise scaling)
- $\mathbf{W}(t)$ is an m-dimensional Wiener process (see subsection 1.4) with:

$$\mathbb{E}[dW_i(t)] = 0, \quad \mathbb{E}[dW_i(t)dW_j(t')] = \delta_{ij}\delta(t - t')dt \tag{28}$$

1.6 Ito's Lemma

- $f(\mathbf{x}, t)$ be a scalar twice-differentiable function
- $\mathbf{x}$ evolves according to an Ito SDE (see subsection 1.5)

The second-order multivariate Taylor series expansion in differential form is given by

$$df = \frac{\partial f}{\partial t}dt + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}dx_i + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \frac{\partial^2 f}{\partial x_i \partial x_j}dx_i dx_j \tag{29}$$

Using $d\mathbf{x}(t) = \mathbf{A}(\mathbf{x}, t)\, dt + \mathbf{B}(\mathbf{x}, t)\, d\mathbf{W}(t)$, we compute:

$$dx_i = A_i dt + \sum_{k=1}^{m} B_{ik} dW_k \tag{30}$$

$$\begin{aligned} dx_i dx_j &= \left(A_i\, dt + \sum_{k=1}^{m} B_{ik}\, dW_k\right)\left(A_j dt + \sum_{l=1}^{m} B_{jl} dW_l\right) &(31)\\ &= \sum_{k=1}^{m} B_{ik}B_{jk}\, dt + (\text{higher-order terms}) &(32)\end{aligned}$$

where $dW_k dW_l = \delta_{kl}dt$ was used and higher-order terms $dtdt, dtdW_k$ were neglected. Substituting back into the original formula for the second-order Taylor series expansion yields

$$\begin{aligned} df &= \frac{\partial f}{\partial t}dt + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}\left(A_i\, dt + \sum_{k=1}^{m} B_{ik}\, dW_k\right) + \frac{1}{2}\sum_{i,j=1}^{n} \frac{\partial^2 f}{\partial x_i \partial x_j}\left(\sum_{k=1}^{m} B_{ik}B_{jk}\right) dt &(33)\\ &= \frac{\partial f}{\partial t}dt + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}\left(A_i\, dt + \sum_{k=1}^{m} B_{ik}\, dW_k\right) + \frac{1}{2}\sum_{i,j=1}^{n} \frac{\partial^2 f}{\partial x_i \partial x_j}dx_i dx_j dt &(34)\end{aligned}$$

or in vector-matrix notation:

$$\begin{aligned} df &= \left(\frac{\partial f}{\partial t} + \nabla f \cdot \mathbf{A} + \frac{1}{2}\mathrm{Tr}\left(\mathbf{B}\mathbf{B}^T\nabla^2 f\right)\right) dt + (\nabla f \cdot \mathbf{B})\, d\mathbf{W} &(35)\\ &= \left(\frac{\partial f}{\partial t} + \frac{1}{2}\mathrm{Tr}\left(\mathbf{B}\mathbf{B}^T\nabla^2 f\right)\right) dt + \nabla f \cdot d\mathbf{x} &(36)\\ &= \frac{\partial f}{\partial t}dt + \frac{1}{2}d\mathbf{x}^T\nabla^2 f\, d\mathbf{x} + \nabla f \cdot d\mathbf{x} &(37)\end{aligned}$$

1.7 Overdamped Langevin Equation

The equivalent Langevin form (derivative form) of the Ito SDE (see subsection 1.5) is called the Ito-Langevin equation. They are exactly the same. An N-dimensional Ito-Langevin equation with state vector $\mathbf{x} = (x_1, ..., x_N)^T$ is given by

$$\dot{\mathbf{x}} = \mathbf{A}(\mathbf{x}, t) + \mathbf{B}(\mathbf{x}, t)\xi(t) \tag{38}$$

where $\xi(t)$ is white Gaussian noise with $\langle \xi_i \rangle = 0$ and $\langle \xi_i(t)\xi_j(t') \rangle = \delta_{ij}\delta(t - t')$. $\mathbf{A}(\mathbf{x}, t)$ is the drift vector and $\mathbf{B}(\mathbf{x}, t)$ is the diffusion (noise) matrix [2]. Note that some papers instead use the diffusion tensor $\mathbf{D}(\mathbf{x}, t) = \mathbf{B}(\mathbf{x}, t)\mathbf{B}(\mathbf{x}, t)/2$ [3].

1.8 Divergence Theorem - Partial Integration

In general, the divergence theorem for a scalar function p and a vector field $\mathbf{F}$ states:

$$\begin{aligned} \int_\Omega \boldsymbol{\nabla} \cdot (\mathbf{F}p) d\mathbf{x} &= \oint_{\partial\Omega} p\mathbf{F}\mathbf{n} dS = 0 && (39) \\ &= \int_\Omega p\boldsymbol{\nabla} \cdot \mathbf{F} d\mathbf{x} + \int_\Omega \mathbf{F} \cdot \boldsymbol{\nabla} p d\mathbf{x} && (40) \end{aligned}$$

The boundary terms vanish since the PDF vanishes at infinity, thus

$$\int_\Omega p\boldsymbol{\nabla} \cdot \mathbf{F} d\mathbf{x} = -\int_\Omega \mathbf{F} \cdot \boldsymbol{\nabla} p d\mathbf{x}. \tag{41}$$

or in summation form:

$$\int_\Omega p \left(\sum_{i=1}^n \frac{\partial F_i}{\partial x_i} \right) d\mathbf{x} = -\int_\Omega \left(\sum_{i=1}^n F_i \frac{\partial p}{\partial x_i} \right) d\mathbf{x} \tag{42}$$

1.9 Langevin equation PDF obeys the Fokker-Planck Equation

Consider a stochastic system described by the overdamped Langevin equation (see subsection 1.7):

$$\dot{\mathbf{x}} = \mathbf{A}(\mathbf{x}, t) + \mathbf{B}(\mathbf{x}, t)\xi(t) \tag{43}$$

The equivalent Ito stochastic differential equation is (see subsection 1.5):

$$d\mathbf{x} = \mathbf{A}(\mathbf{x}, t)dt + \mathbf{B}(\mathbf{x}, t)d\mathbf{W}(t) \tag{44}$$

where $d\mathbf{W}(t)$ is a Wiener process with $\langle dW_i dW_j \rangle = \delta_{ij} dt$.

For any twice-differentiable function $f(\mathbf{x}, t)$, Ito's lemma is (see subsection 1.6):

$$df = \left(\frac{\partial f}{\partial t} + \nabla f \cdot \mathbf{A} + \frac{1}{2} \mathrm{Tr} \left[\mathbf{B}\mathbf{B}^T \nabla^2 f \right] \right) dt + (\nabla f \cdot \mathbf{B})\, d\mathbf{W} \tag{45}$$

Taking the expectation on both sides and noting $\langle d\mathbf{W}(t) \rangle = 0$:

$$\langle df \rangle = \left\langle \frac{\partial f}{\partial t} + \nabla f \cdot \mathbf{A} + \frac{1}{2} \mathrm{Tr} \left[\mathbf{B}\mathbf{B}^T \nabla^2 f \right] \right) \rangle dt \tag{46}$$

The expected value $\langle f \rangle$ and its derivative can also be expressed in terms of the probability density $p(\mathbf{x}, t)$ (see subsection 1.2):

$$\langle f \rangle = \int pf \, d\mathbf{x} \tag{47}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle f \rangle = \int \left(\frac{\partial f}{\partial t} p + f \frac{\partial p}{\partial t} \right) \, d\mathbf{x} \tag{48}$$

Equating both expressions for $\langle df \rangle$ yields:

$$\int \left(\frac{\partial f}{\partial t} p + f \frac{\partial p}{\partial t} \right) \, d\mathbf{x} = \int \left(\frac{\partial f}{\partial t} p + p\mathbf{A} \cdot \nabla f + p\frac{1}{2}\mathrm{Tr}[\mathbf{B}\mathbf{B}^T \nabla^2 f] \right) \, d\mathbf{x} \tag{49}$$

The terms $p\partial f/\partial t$ cancel each other.
Using the divergence theorem (see subsection 1.8), we can simplify the RHS:

1. for $p\mathbf{A} \cdot \nabla f$:

$$\int p\mathbf{A} \cdot \boldsymbol{\nabla} f \, d\mathbf{x} = -\int \boldsymbol{\nabla} \cdot (p\mathbf{A}) f \, d\mathbf{x} \tag{50}$$

2. for $p\frac{1}{2}\mathrm{Tr}[\mathbf{B}\mathbf{B}^T \nabla^2 f]$:

$$\begin{aligned}
\int p\frac{1}{2}\mathrm{Tr}[\mathbf{B}\mathbf{B}^T \nabla^2 f] \, d\mathbf{x} &= \frac{1}{2} \int p(\mathbf{x}, t) \sum_{i,j} (\mathbf{B}\mathbf{B}^T)_{ij} \frac{\partial^2 f}{\partial x_i \partial x_j} d\mathbf{x} &(51)\\
&= -\int \frac{1}{2} \int \sum_{i,j} \frac{\partial}{\partial x_j} \left[p(\mathbf{B}\mathbf{B}^T)_{ij} \right] \frac{\partial f}{\partial x_i} d\mathbf{x} &(52)\\
&= -\int -\frac{1}{2} \int f \sum_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} \left[(\mathbf{B}\mathbf{B}^T)_{ij} p \right] \, d\mathbf{x} &(53)\\
&= \int f \frac{1}{2} \nabla^2 : (\mathbf{B}\mathbf{B}^T p) \, d\mathbf{x} &(54)
\end{aligned}$$

where (:) denotes the double dot product

Substituting both expressions yields

$$\int f \frac{\partial p}{\partial t} d\mathbf{x} = \int f \left(-\boldsymbol{\nabla} \cdot (p\mathbf{A}) + \frac{1}{2} \nabla^2 : (\mathbf{B}\mathbf{B}^T p) \right) \, d\mathbf{x} \tag{55}$$

Because the boundary is infinity but arbitrary

$$f \frac{\partial p}{\partial t} = f \left(-\boldsymbol{\nabla} \cdot (p\mathbf{A}) + \frac{1}{2} \nabla^2 : (\mathbf{B}\mathbf{B}^T p) \right) \tag{56}$$

and because f is also arbitrary

$$\begin{aligned}
\frac{\partial p(\mathbf{x}, t)}{\partial t} &= -\boldsymbol{\nabla} \cdot (p(\mathbf{x}, t)\mathbf{A}(\mathbf{x}, t)) + \frac{1}{2} \nabla^2 : (\mathbf{B}(\mathbf{x}, t)\mathbf{B}(\mathbf{x}, t)^T p(\mathbf{x}, t)) &(57)\\
&= -\sum_{i=1}^{n} \frac{\partial}{\partial x_i} \left[A_i(\mathbf{x}, t) p(\mathbf{x}, t) \right] + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial^2}{\partial x_i \partial x_j} \left[D_{ij}(\mathbf{x}, t) p(\mathbf{x}, t) \right] &(58)
\end{aligned}$$

where $\mathbf{D}(\mathbf{x},t) = \mathbf{B}(\mathbf{x},t)\mathbf{B}(\mathbf{x},t)/2$ is the diffusion tensor, which is usually positive definite. This result is called the Fokker-Planck equation. It can be interpreted as a continuity equation, where the RHS is the probability current:

$$\frac{\partial p}{\partial t} = -\boldsymbol{\nabla} \cdot J(\mathbf{x},t) \tag{59}$$

$$\mathbf{J}(\mathbf{x},t) = p(\mathbf{x},t)\mathbf{A}(\mathbf{x},t)) - \frac{1}{2}\boldsymbol{\nabla} \cdot \left(\mathbf{B}(\mathbf{x},t)\mathbf{B}(\mathbf{x},t)^T p(\mathbf{x},t)\right) \tag{60}$$

The RHS can be divided into a parabolic and a hyperbolic term:

$$\frac{\partial p}{\partial t} = - \underbrace{\nabla \cdot (\mathbf{A}p)}_{\text{hyperbolic drift term}} + \underbrace{\frac{1}{2}\nabla^2 : (\mathbf{B}\mathbf{B}^T p)}_{\text{parabolic diffusion term}} \tag{61}$$

A parabolic equation has smooth, continuous solutions (such as the heat equation). A hyperbolic equation (such as the 1st maxwell equation) also allows discontinuous (singular) solutions, such as the delta function. In the example of the delta function, the system would be deterministic, which produces no entropy.

1.10 Fluctuation-Dissipation Theorem

Assume a classical system with state vector $\mathbf{x}$ that evolves according to the Langevin equation.

In a steady state, the PDF $p_{\text{ss}}(\mathbf{x},t)$ does not change with time - the LHS of the Fokker-Planck equation is equal to 0:

$$\frac{\partial p_{\text{ss}}(\mathbf{x},t)}{\partial t} = 0 = -\boldsymbol{\nabla} \cdot (p_{\text{ss}}(\mathbf{x},t)\mathbf{A}(\mathbf{x},t)) + \frac{1}{2}\nabla^2 : (\mathbf{B}(\mathbf{x},t)\mathbf{B}(\mathbf{x},t)^T p_{\text{ss}}(\mathbf{x},t)) \tag{62}$$

$$:= \boldsymbol{\nabla} \cdot \mathbf{J}_{\text{ss}}(\mathbf{x},t) \tag{63}$$

$$\tag{64}$$

Now further assume that this steady state is an equilibrium steady state (ESS). Then, the PDF follows the Boltzmann statistic (see subsection 1.1) with

$$p_{\text{ESS}}(\mathbf{x},t) = Ce^{-\beta H(\mathbf{x})} = p_{\text{ESS}}(\mathbf{x}) \tag{65}$$

In equilibrium, the probability current vanishes, as the probabilities of all processes and their reverse balance out. This means that

$$\mathbf{J}_{\text{ESS}}(\mathbf{x},t) = p_{\text{ESS}}(\mathbf{x},t)\mathbf{A}(\mathbf{x},t)) - \frac{1}{2}\boldsymbol{\nabla} \cdot \left(\mathbf{B}(\mathbf{x},t)\mathbf{B}(\mathbf{x},t)^T p_{\text{ESS}}(\mathbf{x},t)\right) = 0 \tag{66}$$

Using the product rule and the logarithm-trick from subsection 1.2, we obtain

$$0 = p_{\text{ESS}}(\mathbf{x},t)\mathbf{A}(\mathbf{x},t)) - \frac{1}{2}\boldsymbol{\nabla} \cdot \left(\mathbf{B}(\mathbf{x},t)\mathbf{B}(\mathbf{x},t)^T p_{\text{ESS}}(\mathbf{x},t)\right) \tag{67}$$

$$= p_{\text{ESS}}(\mathbf{x},t)\mathbf{A}(\mathbf{x},t)) - \frac{1}{2}p_{\text{ESS}}(\mathbf{x},t)\mathbf{B}(\mathbf{x},t)\mathbf{B}(\mathbf{x},t)^T\boldsymbol{\nabla}\ln\left(p_{\text{ESS}}(\mathbf{x},t)\right) - \frac{1}{2}p_{\text{ESS}}(\mathbf{x},t)\boldsymbol{\nabla} \cdot \left(\mathbf{B}(\mathbf{x},t)\mathbf{B}(\mathbf{x},t)^T\right)$$

If diffusion is isotropic with $\mathbf{B}(\mathbf{x},t)\mathbf{B}(\mathbf{x},t)^T = \mathbf{B}\mathbf{B}^T = \text{const}$, the expression simplifies to

$$\begin{aligned}\mathbf{A}(\mathbf{x},t)) &= \frac{1}{2}\mathbf{B}\mathbf{B}^T\boldsymbol{\nabla}\ln\left(p_{\text{ESS}}(\mathbf{x},t)\right)\\ &= \frac{1}{2}\mathbf{B}\mathbf{B}^T\boldsymbol{\nabla}\ln\left(Ce^{-\beta H(\mathbf{x})}\right)\\ &= -\frac{\beta}{2}\mathbf{B}\mathbf{B}^T\boldsymbol{\nabla}\left(H(\mathbf{x})\right)\end{aligned} \tag{68}$$

This last result is the statement of the Fluctuation-Dissipation theorem.
Using the Equipartition theorem (see subsection 1.1), we can derive an expression for the diffusion tensor so that the noise is consistent with the Hamiltonian.

1. Assume that $\mathbf{B}$ is a diagonal matrix $\rightarrow \mathbf{D} = \text{diag}(B_1^2, ..., B_m^2)$

For this, take any row k from Equation 68

$$A_k(\mathbf{x}, t)) = -\frac{\beta}{2} B_k^2 \frac{\partial}{\partial x_k} H(\mathbf{x}) \tag{69}$$

and multiply it by x_k:

$$A_k(\mathbf{x}, t)) x_k = -\frac{\beta}{2} B_k^2 x_k \frac{\partial}{\partial x_k} H(\mathbf{x}) \tag{70}$$

Take the expectation on both sides:

$$\langle A_k(\mathbf{x}, t)) x_k \rangle = -\frac{\beta}{2} B_k^2 \left\langle x_k \frac{\partial}{\partial x_k} H(\mathbf{x}) \right\rangle \tag{71}$$

Using the Equipartition theorem (see subsection 1.1) for the RHS yields the equality

$$\langle A_k(\mathbf{x}, t)) x_k \rangle = -\frac{\beta}{2} B_k^2 \frac{1}{\beta} \tag{72}$$

Rearranging and taking the square root:

$$B_k = \sqrt{-2 \langle A_k(\mathbf{x}, t)) x_k \rangle} \tag{73}$$

2 Circuit Theory Stuff

2.1 Node Flux

Define the node flux ϕ, which is connected to the voltage U via

$$\dot{\phi} = U \tag{74}$$

Motivation from 2nd Maxwell equation:

$$\begin{aligned}
\nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} \\
\int_S (\nabla \times \mathbf{E}) \cdot d\mathbf{S} &= \oint_{\partial S} \mathbf{E} \cdot d\mathbf{l} := E \\
&= -\int_S \frac{\partial \mathbf{B}}{\partial t} \cdot d\mathbf{S} = -\frac{\partial}{\partial t} \int_S \mathbf{B} \cdot d\mathbf{S}
\end{aligned}$$

Equations for ohmic resistor, capacitor, coil:

- Ohmic Resistor (dissipates energy $\rightarrow$ no Hamiltonian in the classical sense):

$$\dot{\phi}_{\mathrm{R}} = R I_{\mathrm{R}} = U_{\mathrm{R}} \tag{75}$$

- Coil (stores energy in magnetic field as current I_{L}):

$$\dot{\phi}_{\mathrm{L}} = L \frac{\mathrm{d}I_{\mathrm{L}}}{\mathrm{d}t} = U_{\mathrm{L}} \quad \rightarrow \quad \phi_{\mathrm{L}} = L I_{\mathrm{L}} \tag{76}$$

$$H_{\mathrm{L}} = \frac{1}{2} L I_{\mathrm{L}}^2 = \frac{\phi_{\mathrm{L}}^2}{2L} \tag{77}$$

- Capacitor (stores energy in electric field as charge Q_{C}:

$$I_{\mathrm{C}} = C \ddot{\phi}_{\mathrm{C}} = C \frac{\mathrm{d}U_{\mathrm{C}}}{\mathrm{d}t} \tag{78}$$

$$H_{\mathrm{C}} = \frac{1}{2} C U_{\mathrm{C}}^2 = \frac{Q_{\mathrm{C}}^2}{2C} \tag{79}$$

2.2 Thermal Bath Coupling

$$H_{\mathrm{bath}} = \sum_k \left(\frac{p_k^2}{2m_k} + \frac{1}{2} m_k \omega_k^2 q_k^2 \right) \tag{80}$$

$$= \sum_k \hbar \omega_k \left(a_k^\dagger a_k + \frac{1}{2} \right) \tag{81}$$

$$H_{\mathrm{coupling}} = -A \sum_k c_k q_k \tag{82}$$

$$= A \sum_k g_k \left(b_k^\dagger + b_k \right) \tag{83}$$

3 Minimal Examples

3.1 Pure Diffusion

Consider a one-dimensional system with initial state x_0. The time evolution is governed by an overdamped Langevin equation (see subsection 1.7 with no drift ($\mathbf{A}(\mathbf{x}, t) = 0$) and isotropic diffusion ($\mathbf{B}(\mathbf{x}, t) = B$)

$$\dot{x} = B\xi(t). \tag{84}$$

3.1.1 Computing Mean and Variance via Time integration and Interchangeability of Expectation and Derivative

1. For $\langle x(t) \rangle$:

$$\begin{aligned}
\dot{x}(t) &= B\xi(t) \\
x(t) &= B \int_0^t \xi(t')\, dt' \\
\langle x(t) \rangle &= B \int_0^t \langle \xi(t') \rangle \; dt' = B \int_0^t 0\, dt' = 0
\end{aligned} \tag{85}$$

2. For $\langle x(t) \rangle$:

$$\begin{aligned}
x^2(t) &= \left(B \int_0^t \xi(t')\, dt' \right)^2 = B^2 \int_0^t \int_0^t \xi(t')\xi(t'')\, dt' dt'' \\
\left\langle x^2(t) \right\rangle &= \left\langle B^2 \int_0^t \int_0^t \xi(t')\xi(t'')\, dt' dt'' \right\rangle = B^2 \int_0^t \int_0^t \langle \xi(t')\xi(t'') \rangle \; dt' \; dt'' \\
&= B^2 \int_0^t \int_0^t \delta(t'' - t')\, dt' \; dt'' = B^2 \int_0^t \; dt'' = B^2 t
\end{aligned} \tag{86}$$

The variance is then

$$\langle\langle x(t) \rangle\rangle = \left\langle x^2(t) \right\rangle - \langle x(t) \rangle^2 = B^2 t - 0 = B^2 t \tag{87}$$

Alternatively (**???????**):

$$\begin{aligned}
x(t)\dot{x}(t) &= \frac{1}{2}\frac{\mathrm{d}x^2(t)}{\mathrm{d}t} = B^2 x(t)\xi(t) = B^2 \xi(t) \int_0^t \xi(t')\, dt' \\
x^2(t) &= 2B^2 \int_0^t \int_0^{t''} \xi(t'')\xi(t')\, dt' \; dt'' \\
\left\langle x^2(t) \right\rangle &= 2B^2 \int_0^t \int_0^{t''} \langle \xi(t'')\xi(t') \rangle \; dt' \; dt'' \\
&= 2B^2 \int_0^t \int_0^{t''} \delta(t' - t'')\, dt' \; dt'' = 2B^2 \int_0^t \; dt'' = 2B^2 t\textbf{???????}
\end{aligned} \tag{88}$$

3.1.2 Computing Mean and Variance via Ito's Lemma

Ito's Lemma (see subsection 1.6), applied to a function $f(x)$ for this system is

$$\langle df \rangle = \left\langle \frac{1}{2} B^2 \frac{\mathrm{d}^2 f}{\mathrm{d}x^2} \right\rangle dt \tag{89}$$

Setting $f = x(t)$ and $f = x^2(t)$ and using the interchangeability of expectation and derivative yields

$$\langle dx \rangle = 0 \quad \to \quad \langle x(t) \rangle = x_0 \tag{90}$$

$$\langle dx^2 \rangle = B^2\, dt \quad \to \quad \langle x^2(t) \rangle = x_0^2 + B^2 t \tag{91}$$

$$\to \quad \langle\langle x(t) \rangle\rangle = \langle x^2(t) \rangle - \langle x(t) \rangle^2 = B^2 t \tag{92}$$

3.1.3 Computing Mean and Variance via the Fokker-Planck Equation

The Fokker-Planck equation for this system reads

$$\frac{\partial p(x,t)}{\partial t} = \frac{1}{2} B^2 \frac{\partial^2 p}{\partial x^2} \tag{93}$$

$$p(x,0) = \delta(x - x_0) \tag{94}$$

which is a linear parabolic PDE. Solution:

1. Transform in Fourier space:

$$\hat{p}(\omega, t) = \int_{-\infty}^{\infty} p(x,t) e^{-i\omega x}\, dx \tag{95}$$

$$\hat{p}(\omega, 0) = e^{-i\omega x_0} \tag{96}$$

2. Obtain new PDE in Fourier space and solve via separation of variables:

$$\frac{\partial \hat{p}}{\partial t} = -\frac{1}{2}\omega^2 B^2 \hat{p} \quad \to \quad \hat{p}(\omega, t) = e^{-i\omega x_0} e^{-\frac{1}{2}\omega^2 B^2 t} \tag{97}$$

3. Inverse Fourier transform back into state space

$$p(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega x} e^{-i\omega x_0} e^{-\frac{1}{2}\omega^2 B^2 t}\, d\omega \tag{98}$$

4. perform quadratic completion

$$-\frac{B^2 t}{2}\omega^2 + i\omega(x - x_0) = -\frac{B^2 t}{2}\left(\omega - \frac{i(x-x_0)}{B^2 t}\right)^2 - \frac{(x-x_0)^2}{2B^2 t} \tag{99}$$

and substituting back. By evaluating the error function, we obtain

$$p(x,t) = \frac{1}{2\pi} e^{-\frac{(x-x_0)^2}{2B^2 t}} \int_{-\infty}^{\infty} e^{-\frac{B^2 t}{2}\left(\omega - \frac{i(x-x_0)}{B^2 t}\right)^2}\, d\omega \tag{100}$$

5. Solve integral with error function

$$\int_{-\infty}^{\infty} e^{-az^2} dz = \sqrt{\frac{\pi}{a}} \tag{101}$$

$$\int_{-\infty}^{\infty} e^{-\frac{B^2 t}{2}\left(\omega - \frac{i(x-x_0)}{B^2 t}\right)^2} d\omega = \sqrt{\frac{2\pi}{B^2 t}} \quad \text{with } a = \frac{B^2 t}{2} \tag{102}$$

6. Final solution:

$$p(x,t) = \frac{1}{\sqrt{2\pi B^2 t}} e^{-\frac{(x-x_0)^2}{2B^2 t}} \tag{103}$$

This is the PDF of a Gaussian distribution with

$$\langle x(t) \rangle = x_0 \tag{104}$$

$$\langle\langle x(t) \rangle\rangle = \left\langle x^2(t) \right\rangle - \langle x(t) \rangle^2 = B^2 t \tag{105}$$

3.2 LR Circuit with Current Source

Consider an electrical circuit consisting of

- Ohmic Resistor:

$$\dot{\phi}_\mathrm{R} = R I_\mathrm{R} = U_\mathrm{R} \tag{106}$$

- Coil:

$$\dot{\phi}_\mathrm{L} = L \frac{\mathrm{d}I_\mathrm{L}}{\mathrm{d}t} = U_\mathrm{L} \quad \to \quad \phi_\mathrm{L} = L I_\mathrm{L} \tag{107}$$

- Current Source I_0

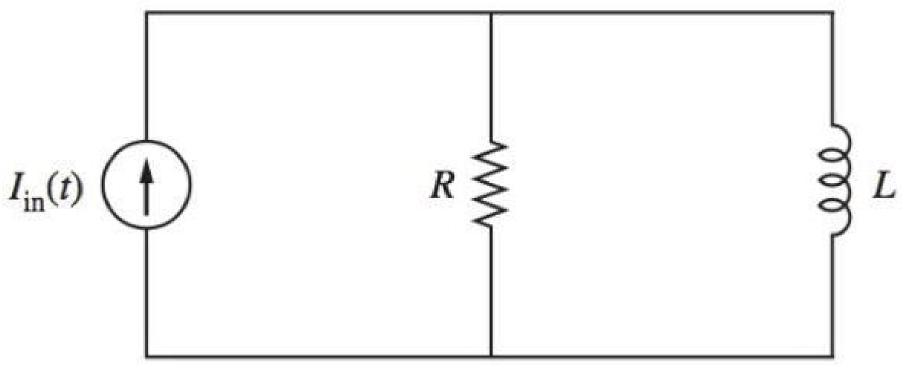

Figure 1: LR Circuit

Kirchhoff's rules yield:

$$U_\mathrm{R} = U_\mathrm{L} \tag{108}$$

$$I_\mathrm{R} + I_\mathrm{L} = I_0 \tag{109}$$

Substituting node flux for current and voltage results in

$$I_{\mathrm{R}} + I_{\mathrm{L}} = \frac{\dot{\phi}_{\mathrm{R}}}{R} + \frac{\phi_{\mathrm{L}}}{L} = I_0 \tag{110}$$

since Maxwell's equations are gauge-invariant, we can say that from $\dot{\phi}_{\mathrm{R}} = \dot{\phi}_{\mathrm{L}} \to \phi_{\mathrm{R}} = \phi_{\mathrm{R}} = \phi$. This results in the ODE

$$\frac{\dot{\phi}}{R} + \frac{\phi}{L} = I_0 \tag{111}$$

Now assume that I_0 is not a current source in the classical sense, but thermal (white) noise $I_0 = B\xi(t)$ due to heat exchange with an infinite heat bath at temperature T. The equation then becomes an overdamped Langevin equation

$$\dot{\phi} = -\frac{R}{L}\phi + B\xi(t). \tag{112}$$

with $A(x,t) = -R\phi/L$.

3.2.1 Determining the value for the Noise Term B consistent with the Equipartition Theorem

In one dimension, we can use the result from the Fluctuation-Dissipation theorem (see Equation 73) to obtain the consistent diffusion term B: With

$$\langle A(x,t))x\rangle = -\left\langle \frac{R}{L}\phi^2 \right\rangle = -2R\left\langle \frac{\phi^2}{2L} \right\rangle = -R\,H_{\mathrm{L}} = -R\left\langle \phi\frac{\mathrm{d}}{\mathrm{d}\phi}\frac{\phi^2}{2L} \right\rangle = -R\left\langle \phi\frac{\mathrm{d}}{\mathrm{d}\phi}H_{\mathrm{L}} \right\rangle \tag{113}$$

Using the Equipartition theorem (see subsection 1.1), the last term is equal to

$$\langle A(x,t))x\rangle = -\frac{R}{\beta} \tag{114}$$

and then using the Fluctuation-Dissipation theorem (see subsection 1.10), we obtain

$$B = \sqrt{-2\,\langle A(,t))x_k\rangle} = \sqrt{2Rk_{\mathrm{B}}T} \tag{115}$$

This result was also derived by Nyquist and Johnson (Johnson-Nyquist noise).

3.2.2 Computing Mean and Variance via Time integration and Interchangeability of Expectation and Derivative

Using the method of variation of constants, the general solution of the LR-ODE is

$$\phi(t) = \phi(0)e^{-\frac{R}{L}t} + B\int_0^t e^{-\frac{R}{L}(t-\tau)}\xi(\tau)\,d\tau \tag{116}$$

Now determine the expected value and the variance:

1. For $\langle\phi(t)\rangle$:

$$\langle\phi(t)\rangle = \left\langle\phi(0)e^{-\frac{R}{L}t}\right\rangle + B\int_0^t \left\langle e^{-\frac{R}{L}(t-\tau)}\xi(\tau)\right\rangle\,d\tau$$

   Since $\langle\cdot\rangle$ is the ensemble average,

$$\begin{aligned}\langle\phi(t)\rangle &= \left\langle\phi(0)e^{-\frac{R}{L}t}\right\rangle + B\int_0^t e^{-\frac{R}{L}(t-\tau)}\left\langle\xi(\tau)\right\rangle\,d\tau = \\ &= \phi(0)e^{-\frac{R}{L}t}\end{aligned} \tag{117}$$

2. For $\langle\phi^2(t)\rangle$:

$$\begin{aligned}\phi^2(t) &= \left(\phi(0)e^{-\frac{R}{L}t} + B\int_0^t e^{-\frac{R}{L}(t-\tau)}\xi(\tau)\,d\tau\right)^2 \\ &= \phi^2(0)e^{-\frac{2R}{L}t} + 2\phi(0)e^{-\frac{R}{L}t}B\int_0^t e^{-\frac{R}{L}(t-\tau)}\xi(\tau)\,d\tau + B^2\int_0^t\int_0^t e^{-\frac{R}{L}(t-\tau)}e^{-\frac{R}{L}(t-\tau')}\xi(\tau)\xi(\tau')\,d\tau\end{aligned}$$

   Taking the expectation on both sides

$$\begin{aligned}\left\langle\phi^2(t)\right\rangle &= \left\langle\phi^2(0)e^{-\frac{2R}{L}t}\right\rangle + B^2\int_0^t\int_0^t e^{-\frac{R}{L}(t-\tau)}e^{-\frac{R}{L}(t-\tau')}\left\langle\xi(\tau)\xi(\tau')\right\rangle\,d\tau d\tau' \\ &= \phi^2(0)e^{-\frac{2R}{L}t} + B^2\int_0^t\int_0^t e^{-\frac{R}{L}(t-\tau)}e^{-\frac{R}{L}(t-\tau')}\delta(\tau-\tau')\,d\tau d\tau' \\ &= \phi^2(0)e^{-\frac{2R}{L}t} + B^2\int_0^t e^{-\frac{2R}{L}(t-\tau)}\,d\tau \\ &= \phi^2(0)e^{-\frac{2R}{L}t} + \frac{B^2L}{2R}\left(1-e^{-\frac{2R}{L}t}\right)\end{aligned} \tag{118}$$

   The variance is then

$$\begin{aligned}\langle\langle\phi(t)\rangle\rangle &= \left\langle\phi^2(t)\right\rangle - \langle\phi(t)\rangle^2 = \phi^2(0)e^{-\frac{2R}{L}t} + \frac{B^2L}{2R}\left(1-e^{-\frac{2R}{L}t}\right) - \phi^2(0)e^{-\frac{2R}{L}t} \\ &= \frac{B^2L}{2R}\left(1-e^{-\frac{2R}{L}t}\right) = k_\mathrm{B}TL\left(1-e^{-\frac{2R}{L}t}\right)\end{aligned} \tag{119}$$

In summary:

$$\langle\phi(t)\rangle = 0 \tag{120}$$

$$\langle\langle\phi^2(t)\rangle\rangle = k_\mathrm{B}TL \tag{121}$$

3.2.3 Computing Mean and Variance via the Fokker-Planck Equation

The Fokker-Planck equation for this system reads

$$\frac{\partial p(\phi,t)}{\partial t} = \frac{R}{L}\frac{\partial}{\partial p}(\phi p) + \frac{1}{2}B^2\frac{\partial^2 p}{\partial \phi^2} \tag{122}$$
$$p(\phi,0) = \delta(\phi - \phi(0)) \tag{123}$$

Linear parabolic PDE: Solve using Fourier Transform

1. Transform in Fourier space:

$$\hat{p}(\omega,t) = \int_{-\infty}^{\infty} p(\phi,t)e^{-i\omega\phi}\,d\phi \tag{124}$$
$$\hat{p}(\omega,0) = e^{-i\omega x_0} \tag{125}$$

2. In Fourier space, the PDE reads:

$$\frac{\partial \tilde{p}}{\partial t} = \frac{R}{L}\left(-i\frac{\partial}{\partial \omega}(\omega\tilde{p}) + \tilde{p}\right) - \frac{1}{2}B^2\omega^2\tilde{p} \tag{126}$$

3. Ansatz:

$$\tilde{p}(\omega,t) = e^{f(\omega,t)} \tag{127}$$

Substituting into PDE in Fourier space, dividing out the exponential terms and solving via separation of variables yields

$$f(\omega,t) = -i\omega\phi(0)e^{-\frac{R}{L}t} - \frac{B^2L}{4R}\omega^2\left(1 - e^{-\frac{2R}{L}t}\right) \tag{128}$$

This form of $f(\omega,t)$ means that $\tilde{p}(\omega,t)$ is gaussian with

$$\mu(t) = \phi(0)e^{-\frac{R}{L}t} \tag{129}$$
$$\sigma^2(t) = \frac{B^2L}{2R}\left(1 - e^{-\frac{2R}{L}t}\right) \tag{130}$$

Since a gaussian in phase space is also a gaussian in Fourier space, we are finished here.

3.3 Resistor with Current Source

Consider an electrical circuit consisting of

- Ohmic Resistor:

$$\dot{\phi}_{\mathrm{R}} = RI_{\mathrm{R}} = U_{\mathrm{R}} \tag{131}$$

- Current Source I_0

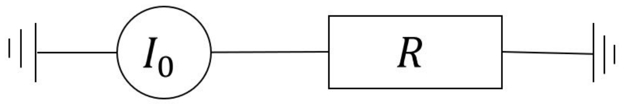

Figure 2: Resistor circuit

By using Kirchhoff's rules, we obtain the ODE

$$I_{\mathrm{R}} = \frac{U_{\mathrm{R}}}{R} = \frac{\dot{\phi}_{\mathrm{R}}}{R} = I_0. \tag{132}$$

Now also take thermal fluctuation $\xi(t)$ into account. Assume that $\xi(t)$ is white noise. The equation then becomes an overdamped Langevin equation (see subsection 1.7)

$$\dot{\phi}_{\mathrm{R}} = RI_0 + B\xi(t) \tag{133}$$

with $A(x,t) = RI_0$.
Since an ohmic resistor does not store energy, a Hamiltonian does not exist for this system. However, since we already derived the noise strength B for the LR circuit, we can use the same value $B = \sqrt{2Rk_{\mathrm{B}}T}$ (see Equation 115).

3.3.1 Computing Mean and Variance via Time integration and Interchangeability of Expectation and Derivative

Integrating both sides with respect to time yields

$$\phi(t) = \int_0^t (RI_0 + B\xi(t'))\,dt' \tag{134}$$

Taking the expectation on both sides yields

$$\langle\phi(t)\rangle = \int_0^t (RI_0 + B\langle\xi(t')\rangle\,dt' = \int_0^t RI_0, dt' \tag{135}$$

The node flux diverges as $t \to \infty$. This result is expected, since there is a never-ending flow of energy into the system.

A References

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