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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 divided by the partition function Z. The probabilites then sum to 1:

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

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 $f(\mathbf{p}, \mathbf{q})$

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

Using partial integration on Equation 3, we obtain

$$\begin{aligned}\frac{1}{Z}\int \frac{\mathrm{d}}{\mathrm{d}x_k}\left(x_k e^{-\beta H(\mathbf{p},\mathbf{q})}\right) d\Gamma &= C\int x_k e^{-\beta H(\mathbf{p},\mathbf{q})}\Big|_a^b d\Gamma_k \\ &= \frac{1}{Z}\int e^{-\beta H(\mathbf{p},\mathbf{q})} d\Gamma + \frac{1}{Z}\int x_k \frac{\mathrm{d}e^{-\beta H(\mathbf{p},\mathbf{q})}}{\mathrm{d}x_k} d\Gamma\end{aligned} \tag{6}$$

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:

$$\frac{1}{Z}\int x_k e^{-\beta H(\mathbf{p},\mathbf{q})}\Big|_a^b d\Gamma_k = 0 \tag{7}$$

$$\begin{aligned}&= \frac{1}{Z}\int e^{-\beta H(\mathbf{p},\mathbf{q})} d\Gamma + \frac{1}{Z}\int x_k \frac{\mathrm{d}e^{-\beta H(\mathbf{p},\mathbf{q})}}{\mathrm{d}x_k} d\Gamma \\ &= 1 - \frac{1}{Z}\int \beta x_k \frac{\partial H(\mathbf{p},\mathbf{q})}{\partial x_k} e^{-\beta H(\mathbf{p},\mathbf{q})} d\Gamma\end{aligned} \tag{8}$$

Rearranging yields

$$\frac{1}{Z}\int x_k \frac{\partial H(\mathbf{p},\mathbf{q})}{\partial x_k} e^{-\beta H(\mathbf{p},\mathbf{q})} x_k d\Gamma = \left\langle x_k \frac{\partial H(\mathbf{p},\mathbf{q})}{\partial x_k} \right\rangle = \frac{1}{\beta} = k_{\mathrm{B}}T \tag{9}$$

This result is called the Equipartition theorem. For a quadratic Hamiltonian, this expression simplifies to $\langle H \rangle = k_{\mathrm{B}}T/2$.
Equipartition theorem assumptions:

1. Classical (Boltzmann statistics)

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

1.1.1 Connection to the Virial Theorem

The Ehrenfest theorem states that for any operator A, the expected value over all states $\psi(t)$ is:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A \rangle_{\psi(t)} = \left\langle \frac{1}{i\hbar}[A,H] \right\rangle_{\psi(t)} + \left\langle \frac{\partial A}{\partial t} \right\rangle_{\psi(t)} \tag{10}$$

1.2 Divergence Theorem - Partial Integration

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

$$\int_{\Omega} \boldsymbol{\nabla} \cdot (\mathbf{f}p) d\mathbf{x} = \oint_{\partial\Omega} p\mathbf{f}\mathbf{n} dS \tag{11}$$

$$= \int_{\Omega} p \boldsymbol{\nabla} \cdot \mathbf{f} d\mathbf{x} + \int_{\Omega} \mathbf{f} \cdot \boldsymbol{\nabla} p d\mathbf{x} \tag{12}$$

The boundary terms must vanish when p is the PDF, thus

$$\int_{\Omega} p \boldsymbol{\nabla} \cdot \mathbf{f} d\mathbf{x} = -\int_{\Omega} \mathbf{f} \cdot \boldsymbol{\nabla} p d\mathbf{x}. \tag{13}$$

or in summation form:

$$\int_{\Omega} p \left(\sum_{i=1}^{n} \frac{\partial f_i}{\partial x_i} \right) d\mathbf{x} = -\int_{\Omega} \left(\sum_{i=1}^{n} f_i \frac{\partial p}{\partial x_i} \right) d\mathbf{x} \tag{14}$$

1.3 Probability Current (NOT FINISHED)

A general probability current is defined as

$$\mathbf{j}(\mathbf{x}) = \int p(\mathbf{x}) W(\mathbf{x}' \mid \mathbf{x}) - p(\mathbf{x}') W(\mathbf{x} \mid \mathbf{x}') d\mathbf{x}' \tag{15}$$

where $W(\mathbf{x}' \mid \mathbf{x})$ is the transition probability kernel of the transition from a state $\mathbf{x} \to \mathbf{x}'$ and $W(\mathbf{x} \mid \mathbf{x}')$ is the transition probability kernel of its reverse $\mathbf{x}' \to \mathbf{x}$. The entries of $W(\mathbf{x}' \mid \mathbf{x})$ are the transition probabilities from state $\mathbf{x}$ to state $\mathbf{x}'$. In equilibrium, the probability current vanishes. This is called detailed balance.
For Markovian processes, the probability density obeys a continuity equation (as probability is locally conserved):

$$\frac{\partial p(\mathbf{x},t)}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{j}(\mathbf{x},t) = 0 \tag{16}$$

1.4 Interchanging Expectation and Derivative

1.4.1 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

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

1.4.2 Ansatz: Leibnitz Rule

Suppose

$$F(t) = \int_\Omega f(x,t)dx \tag{22}$$

We want to evaluate:

$$\frac{dF}{dt} = \frac{d}{dt}\int_\Omega f(x,t)\,dx = \int_\Omega \frac{\partial f(x,t)}{\partial t}dx \tag{23}$$

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

$$F(t) = \int_\Omega p(\mathbf{x},t)g(x)d\mathbf{x} = \langle g(\mathbf{x},t)\rangle \tag{24}$$

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \frac{\mathrm{d}\,\langle g(\mathbf{x}(t))\rangle}{\mathrm{d}t} = \int_\Omega g(\mathbf{x})\frac{\partial p(\mathbf{x},t)}{\partial t}d\mathbf{x} \tag{25}$$

Note that now, the time-dependence is in the PDF.
If the PDF satisfies a continuity equation (see subsection 1.3), the time derivative $\partial_t p(\mathbf{x}, t)$ can be expressed as the divergence of the probability current:

$$\int_\Omega g(\mathbf{x}) \frac{\partial p(\mathbf{x}, t)}{\partial t} d\mathbf{x} = -\int_\Omega g(\mathbf{x}) \boldsymbol{\nabla} \cdot \mathbf{j}(\mathbf{x}, t) d\mathbf{x}$$

Using the divergence theorem and that the integral must vanish at the boundaries, we obtain

$$-\int_\Omega g(\mathbf{x}) \boldsymbol{\nabla} \cdot \mathbf{j}(\mathbf{x}, t) d\mathbf{x} = \int_\Omega \boldsymbol{\nabla} g(\mathbf{x}) \cdot \mathbf{j}(\mathbf{x}, t) d\mathbf{x}$$

We can rewrite this integral by introducing the mean-field-velocity $\mathbf{v}_{mf} \hat{=} \dot{\mathbf{x}}$. This is not equal to $\dot{\mathbf{x}}$, as the time derivative may not exist for stochastic systems, as Wiener processes have infinite variation. Define

$$\mathbf{j}(\mathbf{x}, t) := p(\mathbf{x}, t) \mathbf{v}_{mf}$$

We can then write

$$\frac{\mathrm{d} \langle g(\mathbf{x}(t)) \rangle}{\mathrm{d}t} = \langle \boldsymbol{\nabla} g(\mathbf{x}) \mathbf{v}_{mf} \rangle \hat{=} \left\langle \boldsymbol{\nabla} g(\mathbf{x}) \frac{\partial \mathbf{x}}{\partial t} \right\rangle = \left\langle \frac{\partial g(\mathbf{x})}{\partial t} \right\rangle \tag{26}$$

1.5 Wiener Processes

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

1. Initial condition:
$$w(0) = 0 \quad \text{(almost surely)} \tag{27}$$
2. Independent increments: For any $0 \leq t_1 < t_2 < \cdots < t_n$,
$$w(t_{k+1}) - w(t_k) \text{ are independent random variables} \tag{28}$$
3. Gaussian increments:
$$w(t) - w(s) \sim \mathcal{N}(0, t - s) \quad \text{for } t > s \geq 0 \tag{29}$$
4. Continuous paths:
$$t \mapsto w(t) \text{ is almost surely continuous} \tag{30}$$

1.6 Ito SDE

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

$$d\mathbf{x}(t) = \mathbf{a}(\mathbf{x}, t)\, dt + \mathbf{B}(\mathbf{x}, t)\, d\mathbf{w}(t) \tag{31}$$

where:

- $\mathbf{a} : \mathbb{R}^n \times [0, \infty) \to \mathbb{R}^n$ is the drift vector (deterministic component)
- $\mathbf{B} : \mathbb{R}^n \times [0, \infty) \to \mathbb{R}^{n \times m}$ is the diffusion (noise scaling), which is an $n \times m$ matrix
- $\mathbf{w}(t)$ is an m-dimensional Wiener process (m-dimensional vector) (see subsection 1.5) with:

$$\mathbb{E}[dW_i(t)] = 0, \quad \mathbb{E}[dW_i(t) dW_j(t')] = \delta_{ij} \delta(t - t') dt \tag{32}$$

1.7 Ito's Lemma

- $f(\mathbf{x}, t)$ be a scalar twice-differentiable function
- $\mathbf{x}$ evolves according to an Ito SDE (see subsection 1.6)

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

$$df = \frac{\partial f}{\partial t}dt + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}dx_i + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \frac{\partial^2 f}{\partial x_i \partial x_j}dx_i dx_j \tag{33}$$

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

$$dx_i = a_i dt + \sum_{k=1}^{m} B_{ik} dW_k \tag{34}$$

$$dx_i dx_j = \left(a_i\, dt + \sum_{k=1}^{m} B_{ik}\, dW_k\right)\left(a_j dt + \sum_{l=1}^{m} B_{jl} dW_l\right) \tag{35}$$

$$= \sum_{k=1}^{m} B_{ik} B_{jk}\, dt + \text{(higher-order terms)} \tag{36}$$

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

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

or in vector-matrix notation:

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

1.8 Overdamped Langevin Equation

The equivalent Langevin form (derivative form) of the Ito SDE (see subsection 1.6) 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

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

where $\boldsymbol{\xi}(t)$ 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 $\mathbf{D}(\mathbf{x}, t) = \mathbf{B}(\mathbf{x}, t)\mathbf{B}(\mathbf{x}, t)/2$ [4].

1.9 Langevin equation PDF obeys the Fokker-Planck (Forward Kolmogorov) Equation

Consider a stochastic system described by the overdamped Langevin equation (see subsection 1.8):

$$\dot{\mathbf{x}} = \mathbf{a}(\mathbf{x}, t) + \mathbf{B}(\mathbf{x}, t)\boldsymbol{\xi}(t) \tag{39}$$

The equivalent Ito stochastic differential equation is (see subsection 1.6):

$$d\mathbf{x} = \mathbf{a}(\mathbf{x}, t)dt + \mathbf{B}(\mathbf{x}, t)d\mathbf{w}(t) \tag{40}$$

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 1.7):

$$df = \left(\frac{\partial f}{\partial t} + \nabla f \cdot \mathbf{a} + \frac{1}{2}\mathrm{Tr}\left[\mathbf{B}\mathbf{B}^T \nabla^2 f\right] \right) dt + (\nabla f \cdot \mathbf{B})\, d\mathbf{w} \tag{41}$$

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

$$\langle df \rangle = \left\langle \frac{\partial f}{\partial t} + \nabla f \cdot \mathbf{a} + \frac{1}{2}\mathrm{Tr}\left[\mathbf{B}\mathbf{B}^T \nabla^2 f\right] \right) \rangle dt \tag{42}$$

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 1.4):

$$\langle f \rangle = \int p f \, d\mathbf{x} \tag{43}$$

$$\frac{\mathrm{d}}{\mathrm{dt}}\langle f \rangle = \int \left(\frac{\partial f}{\partial t} p + f \frac{\partial p}{\partial t} \right) d\mathbf{x} \tag{44}$$

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

$$\int \left(\frac{\partial f}{\partial t} p + f \frac{\partial p}{\partial t} \right) d\mathbf{x} = \int \left(\frac{\partial f}{\partial t} p + p\mathbf{a} \cdot \nabla f + p\frac{1}{2}\mathrm{Tr}[\mathbf{B}\mathbf{B}^T \nabla^2 f] \right) d\mathbf{x} \tag{45}$$

The terms $p\partial f/\partial t$ cancel each other.
Using the divergence theorem (see subsection 1.2), we can simplify the RHS:

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

$$\int p\mathbf{a} \cdot \boldsymbol{\nabla} f \, d\mathbf{x} = -\int \boldsymbol{\nabla} \cdot (p\mathbf{a}) f \, d\mathbf{x} \tag{46}$$

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

$$\int p\frac{1}{2}\mathrm{Tr}[\mathbf{B}\mathbf{B}^T\nabla^2 f]\, d\mathbf{x} = \frac{1}{2}\int p(\mathbf{x},t)\sum_{i,j}(\mathbf{B}\mathbf{B}^T)_{ij}\frac{\partial^2 f}{\partial x_i \partial x_j}d\mathbf{x} \tag{47}$$

$$= -\int \frac{1}{2}\int \sum_{i,j}\frac{\partial}{\partial x_j}\left[p(\mathbf{B}\mathbf{B}^T)_{ij}\right]\frac{\partial f}{\partial x_i}d\mathbf{x} \tag{48}$$

$$= -\int -\frac{1}{2}\int f\sum_{i,j}\frac{\partial^2}{\partial x_i \partial x_j}\left[(\mathbf{B}\mathbf{B}^T)_{ij}p\right]d\mathbf{x} \tag{49}$$

$$= \int f\frac{1}{2}\nabla^2 : (\mathbf{B}\mathbf{B}^T p)\, d\mathbf{x} \tag{50}$$

where (:) denotes the double dot product

Substituting both expressions yields

$$\int f\frac{\partial p}{\partial t}d\mathbf{x} = \int f\left(-\boldsymbol{\nabla}\cdot(p\mathbf{a}) + \frac{1}{2}\nabla^2 : (\mathbf{B}\mathbf{B}^T p)\right)d\mathbf{x} \tag{51}$$

Because the boundary is infinity but arbitrary

$$f\frac{\partial p}{\partial t} = f\left(-\boldsymbol{\nabla}\cdot(p\mathbf{a}) + \frac{1}{2}\nabla^2 : (\mathbf{B}\mathbf{B}^T p)\right) \tag{52}$$

and because f is also arbitrary

$$\frac{\partial p(\mathbf{x},t)}{\partial t} = -\boldsymbol{\nabla}\cdot(p(\mathbf{x},t)\mathbf{a}(\mathbf{x},t)) + \frac{1}{2}\nabla^2 : (\mathbf{B}(\mathbf{x},t)\mathbf{B}(\mathbf{x},t)^T p(\mathbf{x},t)) \tag{53}$$

$$= -\sum_{i=1}^{n}\frac{\partial}{\partial x_i}\left[A_i(\mathbf{x},t)p(\mathbf{x},t)\right] + \sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\partial^2}{\partial x_i \partial x_j}\left[D_{ij}(\mathbf{x},t)p(\mathbf{x},t)\right] \tag{54}$$

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:

$$\frac{\partial p}{\partial t} = -\boldsymbol{\nabla}\cdot\mathbf{j}(\mathbf{x},t) \tag{55}$$

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

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

$$\frac{\partial p}{\partial t} = -\underbrace{\nabla\cdot(\mathbf{a}p)}_{\text{hyperbolic drift term}} + \underbrace{\frac{1}{2}\nabla^2 : (\mathbf{B}\mathbf{B}^T p)}_{\text{parabolic diffusion term}} \tag{56}$$

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 Time Evolution of the expected Value of an arbitrary Function

Take any differentiable function $\phi(\mathbf{x})$. Using Ito's Lemma, we obtain

$$d\phi = \left(\frac{\partial \phi}{\partial t} + \nabla\phi \cdot \mathbf{a} + \frac{1}{2}\mathrm{Tr}\left(\mathbf{B}\mathbf{B}^T\nabla^2\phi\right)\right) dt + \left(\nabla\phi \cdot \mathbf{B}\right) d\mathbf{w}$$

taking the expected value on both sides:

$$\begin{aligned}\langle d\phi\rangle &= \left\langle \left(\frac{\partial \phi}{\partial t} + \nabla\phi \cdot \mathbf{a} + \frac{1}{2}\mathrm{Tr}\left(\mathbf{B}\mathbf{B}^T\nabla^2\phi\right)\right) dt \right\rangle + \left\langle \left(\nabla\phi \cdot \mathbf{B}\right) d\mathbf{w}\right\rangle \\ &= \left\langle \left(\frac{\partial \phi}{\partial t} + \nabla\phi \cdot \mathbf{a} + \frac{1}{2}\mathrm{Tr}\left(\mathbf{B}\mathbf{B}^T\nabla^2\phi\right)\right)\right\rangle dt\end{aligned}$$

Integrating on both sides:

$$\langle \phi(\mathbf{x}(T))\rangle = \langle \phi(\mathbf{x}(0))\rangle + \int_0^T \left\langle \left(\frac{\partial \phi}{\partial t} + \nabla\phi \cdot \mathbf{a} + \frac{1}{2}\mathrm{Tr}\left(\mathbf{B}\mathbf{B}^T\nabla^2\phi\right)\right)\right\rangle dt \tag{57}$$

And the time derivative:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \phi(\mathbf{x}(t))\rangle = \left\langle \left(\frac{\partial \phi}{\partial t} + \nabla\phi \cdot \mathbf{a} + \frac{1}{2}\mathrm{Tr}\left(\mathbf{B}\mathbf{B}^T\nabla^2\phi\right)\right)\right\rangle \tag{58}$$

1.11 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 $p_{\mathrm{ss}}(\mathbf{x}, t)$ does not change with time - the LHS of the Fokker-Planck equation is equal to 0:

$$\begin{aligned}\frac{\partial p_{\mathrm{ss}}(\mathbf{x}, t)}{\partial t} &= 0 = -\boldsymbol{\nabla} \cdot \left(p_{\mathrm{ss}}(\mathbf{x}, t)\mathbf{a}(\mathbf{x}, t)\right) + \frac{1}{2}\nabla^2 : \left(\mathbf{B}(\mathbf{x}, t)\mathbf{B}(\mathbf{x}, t)^T p_{\mathrm{ss}}(\mathbf{x}, t)\right) \\ &:= \boldsymbol{\nabla} \cdot \mathbf{j}_{\mathrm{ss}}(\mathbf{x}, t)\end{aligned}$$

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

$$p_{\mathrm{ESS}}(\mathbf{x}, t) = Ce^{-\beta H(\mathbf{x})} = p_{\mathrm{ESS}}(\mathbf{x}) \tag{59}$$

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

$$\mathbf{j}_{\mathrm{ESS}}(\mathbf{x}, t) = p_{\mathrm{ESS}}(\mathbf{x}, t)\mathbf{a}(\mathbf{x}, t)) - \frac{1}{2}\boldsymbol{\nabla} \cdot \left(\mathbf{B}(\mathbf{x}, t)\mathbf{B}(\mathbf{x}, t)^T p_{\mathrm{ESS}}(\mathbf{x}, t)\right) = 0$$

Using the product rule and the nice trick

$$\frac{\partial p_{\mathrm{ESS}}(\mathbf{x}, t)}{\partial t} = p_{\mathrm{ESS}}(\mathbf{x}, t)\boldsymbol{\nabla}\ln(p_{\mathrm{ESS}}(\mathbf{x}, t)),$$

to obtain a linear term in $p_{\text{ESS}}(\mathbf{x}, t)$, we get

$$
\begin{aligned}
0 &= p_{\text{ESS}}(\mathbf{x}, t)\mathbf{a}(\mathbf{x}, t)) - \frac{1}{2}\boldsymbol{\nabla} \cdot \left(\mathbf{B}(\mathbf{x}, t)\mathbf{B}(\mathbf{x}, t)^T p_{\text{ESS}}(\mathbf{x}, t)\right) \\
&= p_{\text{ESS}}(\mathbf{x}, t)\mathbf{a}(\mathbf{x}, t)) - \frac{1}{2}p_{\text{ESS}}(\mathbf{x}, t)\mathbf{B}(\mathbf{x}, t)\mathbf{B}(\mathbf{x}, t)^T\boldsymbol{\nabla} \ln\left(p_{\text{ESS}}(\mathbf{x}, t)\right) - \frac{1}{2}p_{\text{ESS}}(\mathbf{x}, t)\boldsymbol{\nabla} \cdot \left(\mathbf{B}(\mathbf{x}, t)\mathbf{B}(\mathbf{x}, t)^T\right)
\end{aligned}
$$

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

$$
\begin{aligned}
\mathbf{a}(\mathbf{x}, t)) &= \frac{1}{2}\mathbf{B}\mathbf{B}^T\boldsymbol{\nabla} \ln\left(p_{\text{ESS}}(\mathbf{x}, t)\right) \\
&= \frac{1}{2}\mathbf{B}\mathbf{B}^T\boldsymbol{\nabla} \ln\left(Ce^{-\beta H(\mathbf{x})}\right) \\
&= -\frac{\beta}{2}\mathbf{B}\mathbf{B}^T\boldsymbol{\nabla}\left(H(\mathbf{x})\right)
\end{aligned}
\tag{60}
$$

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 60

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

and multiply it by x_k:

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

Take the expectation on both sides:

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

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

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

Rearranging and taking the square root:

$$B_k = \sqrt{-2\left\langle a_k(\mathbf{x}, t))x_k\right\rangle} \tag{61}$$

2 TUR

2.1 Entropy production rate

2.1.1 System Entropy production Rate

Gibbs entropy is defined as

$$S_{\text{sys}}(t) = -k_{\text{B}} \int p(\mathbf{x}, t) \ln(p(\mathbf{x}, t))\, d\mathbf{x}$$

Taking the time derivative and pulling the derivative under the integral via Leibniz' rule:

$$\dot{S}_{\text{sys}}(t) = -k_{\text{B}} \int \frac{\partial p(\mathbf{x}, t)}{\partial t} \ln(p(\mathbf{x}, t)) + \frac{\partial p(\mathbf{x}, t)}{\partial t}\, d\mathbf{x}$$

Since integration and differentiation commute, the second integral vanishes:

$$\int \frac{\partial p(\mathbf{x}, t)}{\partial t}\, d\mathbf{x} = \frac{\partial}{\partial t} \int p(\mathbf{x}, t)\, d\mathbf{x} = \frac{\partial}{\partial t}(1) = 0 \tag{62}$$

so we are left with:

$$\boxed{\dot{S}_{\text{sys}}(t) = -k_{\text{B}} \int \frac{\partial p(\mathbf{x}, t)}{\partial t} \ln(p(\mathbf{x}, t))\, d\mathbf{x}} \tag{63}$$

2.1.2 Environment Entropy Production Rate (NOT FINISHED)

The environment's entropy production rate is given by

$$\dot{S}_{\text{env}} = \frac{1}{T} \int \mathbf{j}(\mathbf{x}, t) \cdot \mathbf{f}(\mathbf{x}, t)\, d\mathbf{x} \tag{64}$$

where $\mathbf{F}(\mathbf{x}, t)$ is the thermodynamic force. The total entropy production rate is

$$\dot{S}_{\text{tot}} = \int -k_{\text{B}} \frac{\partial p(\mathbf{x}, t)}{\partial t} \ln(p(\mathbf{x}, t)) + \frac{1}{T} \int \mathbf{j}(\mathbf{x}, t) \cdot \mathbf{f}(\mathbf{x}, t)\, d\mathbf{x}$$

use the continuity equation and express the time derivative of $p(\mathbf{x}, t)$ as the divergence of probability current:

$$= \int k_{\text{B}} \boldsymbol{\nabla} \cdot \mathbf{j}(\mathbf{x}, t) \ln(p(\mathbf{x}, t)) + \frac{1}{T} \int \mathbf{j}(\mathbf{x}, t) \cdot \mathbf{f}(\mathbf{x}, t)\, d\mathbf{x}$$

Using integration by parts (see subsection 1.2) to exchange the divergence with a gradient, we obtain

$$\begin{aligned} \dot{S}_{\text{tot}} &= -k_{\text{B}} \int \mathbf{j}(\mathbf{x}, t) \boldsymbol{\nabla} \ln(p(\mathbf{x}, t)) + \frac{1}{T} \int \mathbf{j}(\mathbf{x}, t) \cdot \mathbf{f}(\mathbf{x}, t)\, d\mathbf{x} \\ &= \int \mathbf{j}(\mathbf{x}, t) \cdot \left(-k_{\text{B}} \frac{\boldsymbol{\nabla} p(\mathbf{x}, t)}{p(\mathbf{x}, t)} + \frac{1}{T} \mathbf{f}(\mathbf{x}, t) \right) d\mathbf{x} \end{aligned} \tag{65}$$

2.1.3 Entropy production rate for an overdamped Langevin System (NOT FINISHED)

The probability current of a system whose time evolution is governed by an overdamped Langevin equation (see subsection 1.8) is obtained from the Fokker-Planck equation (see Equation 55):

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

Assume that the diffusion tensor is constant. In thermal equilibrium relates mobility and diffusion via $\boldsymbol{\mu} = k_\mathrm{B}T\,\mathbf{D}$ where $\boldsymbol{\mu}$ is the mobility tensor and $\mathbf{D} = \mathbf{B}\mathbf{B}^T/2$ is the diffusion tensor. The probability flux can then be expressed as

$$\mathbf{j}(\mathbf{x},t) = \boldsymbol{\mu}\left(p(\mathbf{x},t)\tilde{\mathbf{a}}(\mathbf{x},t) - k_\mathrm{B}T\boldsymbol{\nabla}p(\mathbf{x},t)\right)$$

In this case, the thermodynamic force is the drift $\mathbf{a}(\mathbf{x},t)$. Substituting the expression for the probability current into Equation 65 yields:

$$\begin{aligned}\dot{S}_\mathrm{tot} = \int &\boldsymbol{\mu}\left(p(\mathbf{x},t)\mathbf{a}(\mathbf{x},t) - k_\mathrm{B}T\boldsymbol{\nabla}p(\mathbf{x},t)\right)\\ &\cdot\left(-k_\mathrm{B}\frac{\boldsymbol{\nabla}p(\mathbf{x},t)}{p(\mathbf{x},t)} + \frac{1}{T}\mathbf{a}(\mathbf{x},t)\right)\,d\mathbf{x}\end{aligned}$$

Rearranging the equation for the probability current, we obtain an expression for $\mathbf{a}(\mathbf{x},t)$:

$$\mathbf{a}(\mathbf{x},t) = \frac{\mathbf{j}(\mathbf{x},t)}{p(\mathbf{x},t)} + \frac{1}{2p(\mathbf{x},t)}\boldsymbol{\nabla}\cdot\left(\mathbf{B}(\mathbf{x},t)\mathbf{B}(\mathbf{x},t)^T p(\mathbf{x},t)\right)$$

Now assume that the drift $\mathbf{B}(\mathbf{x},t)$ is constant. Rewrite equations in terms of drift tensor $\mathbf{D} = \mathbf{B}\mathbf{B}^T/2$:

$$\begin{aligned}\dot{S}_\mathrm{tot} &= \int \left(p(\mathbf{x},t)\left(\frac{\mathbf{j}(\mathbf{x},t)}{p(\mathbf{x},t)} + \mathbf{D}\frac{\boldsymbol{\nabla}p(\mathbf{x},t)}{p(\mathbf{x},t)}\right) - \mathbf{D}\boldsymbol{\nabla}p(\mathbf{x},t)\right)\\ &\qquad\cdot\left(-k_\mathrm{B}\frac{\boldsymbol{\nabla}p(\mathbf{x},t)}{p(\mathbf{x},t)} + \frac{1}{T}\left(\frac{\mathbf{j}(\mathbf{x},t)}{p(\mathbf{x},t)} + \mathbf{D}\frac{\boldsymbol{\nabla}p(\mathbf{x},t)}{p(\mathbf{x},t)}\right)\right)\,d\mathbf{x}\\ &= \int \frac{\mathbf{j}(\mathbf{x},t)}{p(\mathbf{x},t)}\cdot\left(-k_\mathrm{B}\boldsymbol{\nabla}p(\mathbf{x},t) + \frac{1}{T}\left(\mathbf{j}(\mathbf{x},t) + \mathbf{D}\boldsymbol{\nabla}p(\mathbf{x},t)\right)\right)\,d\mathbf{x} \qquad (66)\\ & \qquad (67)\end{aligned}$$

2.2 First Proof (Markov Jump Processes) [1]

2.2.1 Key Assumptions

1. **Markov Jump Process**: The system is modeled as a continuous-time Markov jump process with states $x = 1, \dots, N$ and transition rates $r(y, z)$. The process is assumed to be **ergodic** (unique steady state $\pi(x)$) and satisfy **local detailed balance**:
$$F(y, z) = \ln \left(\frac{\pi(y) r(y, z)}{\pi(z) r(z, y)} \right),$$
where $F(y, z)$ is the thermodynamic force (dissipation per transition).

2. **Empirical Current**: The net number of transitions $J_T(y, z)$ along each edge (y, z) is measured over time T. The empirical current $j_T(y, z) = J_T(y, z)/T$ fluctuates around its steady-state value $j^\pi(y, z)$.

3. **Large Deviation Principle (LDP)**: Current fluctuations are exponentially rare, with a probability density $P(J_T = Tj) \sim e^{-TI(j)}$, where $I(j)$ is the **rate function**.

2.2.2 Derivation Steps

2.2.3 Step 1: Bounding the Rate Function

The authors derive two inequalities for the rate function $I(j)$:

1. **Linear-Response (LR) Bound** (Eq. 3 in the paper):
$$I(j) \leq \sum_{y<z} \frac{(j(y, z) - j^\pi(y, z))^2}{4 j^\pi(y, z)} \sigma^\pi(y, z),$$
where $\sigma^\pi(y, z) = j^\pi(y, z) F(y, z)$ is the entropy production rate per edge.
   - This bound is tight near equilibrium (small fluctuations) and saturates at $j = \pm j^\pi$.

2. **Weakened Linear-Response (WLR) Bound** (Eq. 4): For a generalized current $j_d = \sum_{y<z} d(y, z) j(y, z)$, the bound simplifies to:
$$I(j_d) \leq \frac{(j_d - j_d^\pi)^2}{4 (j_d^\pi)^2} \Sigma^\pi,$$
where $\Sigma^\pi = \sum_{y<z} \sigma^\pi(y, z)$ is the **total entropy production rate**.
   - This bound depends only on the total dissipation Σ^π, not individual edge contributions.

2.2.4 Step 2: Connecting to the TUR

The TUR is derived from the **second derivative** of the rate function $I(j_d)$ at $j_d = j_d^\pi$:

1. The variance of j_d is related to the curvature of $I(j_d)$:
$$\mathrm{Var}(j_d) = \frac{1}{I''(j_d^\pi)}.$$

2. Evaluating the second derivative of the WLR bound (Eq. 4) at $j_d = j_d^\pi$ gives:

$$I''(j_d^\pi) \geq \frac{1}{2} \frac{\Sigma^\pi}{(j_d^\pi)^2}.$$

3. Substituting into the variance yields:

$$\mathrm{Var}(j_d) \leq \frac{2(j_d^\pi)^2}{\Sigma^\pi}.$$

4. Rearranging gives the **Thermodynamic Uncertainty Relation (TUR)**:

$$\frac{\mathrm{Var}(j_d)}{(j_d^\pi)^2} \Sigma^\pi \geq 2,$$

or equivalently, the **relative uncertainty** $\epsilon_d^2 = \mathrm{Var}(j_d)/(j_d^\pi)^2$ satisfies:

$$\epsilon_d^2 \Sigma^\pi \geq 2.$$

2.2.5 Step 3: Tightness of the Bound

- The bound is **tightest** in the linear-response regime (near equilibrium) and when the generalized current j_d is proportional to the entropy production rate Σ.
- For other currents, the bound still holds but may not be saturated.

2.2.6 Key Implications

1. **Fundamental Trade-Off**: The TUR shows that reducing current fluctuations (precision) requires increasing dissipation (energy cost). This has implications for designing efficient molecular machines or biochemical networks.
2. **Universality**: The bound applies to **any Markov jump process** with a steady state, including models of molecular motors, chemical reactions, and particle transport (e.g., ASEP).
3. **Link to Fluctuation Theorems**: The symmetry $I(j) = I(-j) - \langle j, F \rangle$ (from fluctuation theorems) ensures the bound is saturated at $j = \pm j^\pi$.

2.2.7 Summary of Derivation

1. Start with the large deviation principle for empirical currents in Markov jump processes.
2. Bound the rate function $I(j)$ using quadratic approximations (LR and WLR bounds).
3. Relate the curvature of $I(j_d)$ to the variance of j_d.
4. Combine with the total entropy production Σ^π to derive the TUR.

The TUR emerges as a **universal constraint** on nonequilibrium fluctuations, linking dissipation, current, and noise in a simple inequality.

2.3 Information theoretic approach (Cramer-Rao and Fisher Information [2]

2.3.1 Assumptions

- The system dynamics are governed by an N-dimensional Itô Langevin equation:

$$\dot{x} = A_\theta(x,t) + \sqrt{2}C(x,t)\xi(t)$$

  where $\xi(t)$ is Gaussian white noise and A_θ depends on a parameter θ to be estimated.

- The stochastic trajectory $x(t)$ is used to define an estimator $\Theta(\Gamma)$ for a function $\psi(\theta)$, where Γ is the trajectory.

- $\Theta(\Gamma)$ is assumed to be an unbiased estimator, i.e., $\langle\Theta(\Gamma)\rangle_\theta = \psi(\theta)$.

- The probability distribution of trajectories $P_\theta(\Gamma)$ is smooth and differentiable in θ.

- The Fisher information is well-defined and finite:

$$I(\theta) = \left\langle \left(\frac{\partial}{\partial\theta} \ln P_\theta(\Gamma) \right)^2 \right\rangle_\theta$$

- Near-equilibrium and additive noise assumptions are made in some cases to simplify expressions (e.g., constant diffusion matrix $B = D\mathbb{I}$).

2.3.2 Derivation Steps Summary

1. Starting from the Cramér-Rao inequality:

$$\mathrm{Var}_\theta[\Theta(\Gamma)] \geq \frac{(\partial_\theta\langle\Theta\rangle_\theta)^2}{I(\theta)}$$

2. Express the Fisher information using a path-integral representation of $P_\theta(\Gamma)$:

$$\ln P_\theta(\Gamma) = \ln\mathcal{N} - \frac{1}{4}\int_0^T (\dot{x} - A_\theta)^T B^{-1}(\dot{x} - A_\theta)\, dt$$

3. Compute the second derivative of the log-likelihood with respect to θ and take its expectation:

$$I(\theta) = -\left\langle \frac{\partial^2}{\partial\theta^2} \ln P_\theta(\Gamma) \right\rangle_\theta$$

4. In the special case of small θ perturbation, derive the fluctuation-response inequality as:

$$\frac{\mathrm{Var}_{\theta=0}[\Theta(\Gamma)]}{[\langle\Theta\rangle_\theta - \langle\Theta\rangle_0]^2} \geq \frac{1}{\theta^2 I(0)}$$

5. Apply this to the integrated current observable $\Theta_{\mathrm{cur}}(\Gamma) = \int_0^T \Lambda(x) \circ \dot{x} dt$ to obtain the thermodynamic uncertainty relation:

$$\frac{\mathrm{Var}[\Theta_{\mathrm{cur}}]}{\langle\Theta_{\mathrm{cur}}\rangle^2} \geq \frac{2}{\langle\dot{S}_{\mathrm{tot}}\rangle T}$$

6. Show that the total entropy production corresponds to the Fisher information in this context.

7. Extend the result using the Chapman-Robbins inequality to non-infinitesimal θ:

$$\frac{\mathrm{Var}_{\theta=0}[\Theta(\Gamma)]}{[\langle\Theta\rangle_\theta - \langle\Theta\rangle_0]^2} \geq \frac{1}{D_{\mathrm{PE}}(P_\theta||P_0)}$$

   where D_{PE} is the Pearson divergence. Generalizable via Chapman-Robins inequality

3 Circuit Theory Stuff

3.1 Node Flux

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

$$\dot{\phi} = U \tag{68}$$

Motivation from 2nd Maxwell equation:

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

Equations for ohmic resistor, capacitor, coil:

- Ohmic Resistor (dissipates energy → no Hamiltonian in the classical sense):

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

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

$$\begin{aligned}
\dot{\phi}_{\mathrm{L}} &= L \frac{\mathrm{d}I_{\mathrm{L}}}{\mathrm{d}t} = U_{\mathrm{L}} \quad \rightarrow \quad \phi_{\mathrm{L}} = L I_{\mathrm{L}} \\
H_{\mathrm{L}} &= \frac{1}{2} L I_{\mathrm{L}}^2 = \frac{\phi_{\mathrm{L}}^2}{2L}
\end{aligned}$$

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

$$\begin{aligned}
I_{\mathrm{C}} &= C \ddot{\phi}_{\mathrm{C}} = C \frac{\mathrm{d}U_{\mathrm{C}}}{\mathrm{d}t} \\
H_{\mathrm{C}} &= \frac{1}{2} C U_{\mathrm{C}}^2 = \frac{Q_{\mathrm{C}}^2}{2C}
\end{aligned}$$

- Josephson Junction stores energy in electric field as charge (Cooper pairs) + coupling potential:

$$\begin{aligned}
I &= I_{\mathrm{c}} \sin\left(\frac{2e}{\hbar}\phi\right) \\
\dot{\phi} &= V \\
H_{\mathrm{JJ}} &= \frac{(2en)^2}{2C} - \frac{\hbar I_{\mathrm{c}}}{2e} \cos\left(\frac{2e}{\hbar}\phi\right)
\end{aligned}$$

3.2 Thermal Bath Coupling

$$\begin{aligned}
H_{\mathrm{bath}} &= \sum_k \left(\frac{p_k^2}{2m_k} + \frac{1}{2} m_k \omega_k^2 q_k^2\right) && (69) \\
&= \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2}\right) && (70)
\end{aligned}$$

$$
\begin{aligned}
H_{\text{coupling}} &= -A \sum_k c_k q_k && (71) \\
&= A \sum_k g_k \left(b_k^\dagger + b_k \right) && (72)
\end{aligned}
$$

4 Numerical Methods for Solving the Ito SDE

Consider the Ito SDE (see subsection 1.6) where the drift and the diffusion term are not explicitely time-dependent with $\mathbf{a}(\mathbf{x}(t)) = \mathbf{a}(\mathbf{x}(t)) = \mathbf{a}(\mathbf{x})$ and $\mathbf{B}(\mathbf{x}(t)) = \mathbf{B}(\mathbf{x}(t)) = \mathbf{B}(\mathbf{x})$:

$$d\mathbf{x}(t) = \mathbf{a}(\mathbf{x})\,dt + \mathbf{B}(\mathbf{x})\,d\mathbf{w}(t).$$

The exact solution over a time interval $[t_n, t_n + \Delta t]$ can be written in integral form:

$$\mathbf{x}(t_{n+1}) = \mathbf{x}(t_n) + \int_{t_n}^{t_n+\Delta t} \mathbf{a}(\mathbf{x}(t))dt + \int_{t_n}^{t_n+\Delta t} \mathbf{B}(\mathbf{x}(t))d\mathbf{w}(t)$$

Or in index form

$$x_i(t_{n+1}) = x_i(t_n) + \int_{t_n}^{t_n+\Delta t} a_i(\mathbf{x}(t))dt + \sum_{j=1}^{M} \int_{t_n}^{t_n+\Delta t} B_{ij}(\mathbf{x}(t))dw_j(t) \tag{73}$$

1. A continuous solution exists when the growth condition is satisfied. This ensures that there is no blow-up in finite time:

$$\|\mathbf{a}(\mathbf{x})\|^2 \leq K_{\mathbf{a}}(1 + \|\mathbf{x}\|^2) \tag{74}$$
$$\|\mathbf{B}(\mathbf{x})\|^2 \leq K_{\mathbf{B}}(1 + \|\mathbf{x}\|^2) \tag{75}$$

2. The solution is unique when the Lipschitz condition (according to the Picard-Lindelöf theorem) is satisfied:

$$\|\mathbf{a}(\mathbf{x}) - \mathbf{a}(\mathbf{y})\| \leq L_{\mathbf{a}}\|\mathbf{x} - \mathbf{y}\|$$
$$\|\mathbf{B}(\mathbf{x}) - \mathbf{B}(\mathbf{y})\| \leq L_{\mathbf{B}}\|\mathbf{x} - \mathbf{y}\|$$

Solutions to physical systems typically remain finite and follow unique paths, hence we can assume that condition 1 and 2 are always fulfilled.

4.1 Convergence

4.1.1 Strong Convergence (Pathwise)

Strong convergence assesses the accuracy of approximating individual sample paths. A numerical method has strong convergence of order γ if

$$\boxed{\mathbb{E}\left[\|\mathbf{x}(t_n) - \mathbf{x}_n\|\right] = \mathcal{O}(\Delta t^{\gamma})} \tag{76}$$

where $x(t_n)$ is the exact solution at time t_n and x_n is the approximate solution at $t_n = \tau$ [3].

4.1.2 Weak Convergence (Distributional)

Weak convergence assesses the accuracy of assessing expectations of functionals of the solution. A numerical method has weak convergence of order β if for all smooth test functions ϕ it satisfies

$$\boxed{|\mathbb{E}[\phi(\mathbf{x}(t_n))] - \mathbb{E}[\phi(\mathbf{x}_n)]| = \mathcal{O}(\Delta t^{\beta})} \tag{77}$$

where $x(t_n)$ is the exact solution at time t_n and x_n is the approximate solution at $t_n = \tau$ [3].

4.2 Euler-Maruyama (Euler-Forward)

Solve the integrals from Equation 73 over a time interval $[t_n, t_n + \Delta t]$. Approximate $a_i(\mathbf{x}) \approx a_i(\mathbf{x}(t_n))$ and $B_{ij}(\mathbf{x}) \approx B_{ij}(\mathbf{x}(t_n))$ up to 0th order:

$$\begin{aligned} x_i(t_n + \Delta t) &\approx x_i(t_n) + \int_{t_n}^{t_n+\Delta t} a_i(\mathbf{x}(t_n))d\tau + \sum_{j=1}^{M} \int_{t_n}^{t_n+\Delta t} B_{ij}(\mathbf{x}(t_n))dw_j(\tau) \\ &= x_i(t_n) + a_i(\mathbf{x}(t_n))\Delta t + \sum_{j=1}^{M} B_{ij}(\mathbf{x}(t_n))\left(w_j(t_n + \Delta t) - w_j(t_n)\right) \end{aligned} \tag{78}$$

After rearranging, we obtain the Euler-Maruyama scheme in both index and vector notation:

$$x_i^{n+1} = x_i^n + a_i(\mathbf{x}_n)\,\Delta t + \sum_{j=1}^{M} B_{ij}(\mathbf{x}_n)\left(w_j^{n+1} - w_j^n\right) \tag{79}$$

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \mathbf{a}(\mathbf{x}_n)\,\Delta t + \mathbf{B}(\mathbf{x}_n)\;(\mathbf{w}_{n+1} - \mathbf{w}_n) \tag{80}$$

Note that since $dw_i dw_j = \delta_{ij}dt$ (see subsection 1.7), $\Delta w_j = \sqrt{\Delta t}$. The Euler-Maruyama method therefore only has strong convergence of order $\gamma = 0.5$, which is limited by the approximation of the diffusion integral. The order of convergence can be improved by expanding $a_i(\mathbf{x})$ and $B_{ij}(\mathbf{x})$ up to a higher order, where Milstones's method comes into play.

4.2.1 Strong Convergence Order (IN BA: ONLY DRIFT <= 0 → evaluate again!!)

The error at t_{n+1} is

$$\begin{aligned} \mathbf{e}_{n+1} &= \mathbf{x}(t_{n+1}) - \mathbf{x}_{n+1} \\ &= \mathbf{x}(t_n) + \int_{t_n}^{t_n+\Delta t} \mathbf{a}(\mathbf{x}(t))dt + \int_{t_n}^{t_n+\Delta t} \mathbf{B}(\mathbf{x}(t))d\mathbf{w}(t) \\ &\quad - \left[\mathbf{x}_n + \mathbf{a}(\mathbf{x}_n)\,\Delta t + \mathbf{B}(\mathbf{x}_n)\;(\mathbf{w}_{n+1} - \mathbf{w}_n)\right] \\ &= \mathbf{e_n} + \mathbf{u}_n + \mathbf{v}_n \end{aligned}$$

where $\mathbf{x}(t_n)$ is the exact solution and $\mathbf{x}_n$ is the approximate solution at time t_n. Next, to make the calculations more readable, define the local errors

$$\begin{aligned} \mathbf{u}_n &:= \int_{t_n}^{t_n+\Delta t} \mathbf{a}(\mathbf{x}(t))dt - \mathbf{a}(\mathbf{x}_n)\,\Delta t \\ \mathbf{v}_n &:= \int_{t_n}^{t_n+\Delta t} \mathbf{B}(\mathbf{x}(t))d\mathbf{w}(t) - \mathbf{B}(\mathbf{x}_n)\;(\mathbf{w}_{n+1} - \mathbf{w}_n)\,. \end{aligned}$$

The expectation of the squared error becomes

$$\begin{aligned} \mathbb{E}\left[\|\mathbf{e}_{n+1}\|^2\right] &= \mathbb{E}\left[\|\mathbf{e}_n + \mathbf{u}_n + \mathbf{v}_n\|^2\right] \\ &= \mathbb{E}\left[\|\mathbf{e}_n\|^2 + 2\mathbf{e}_n \cdot \mathbf{u}_n + 2\mathbf{e}_n \cdot \mathbf{v}_n + \|\mathbf{u}_n\|^2 + 2\mathbf{u}_n \cdot \mathbf{v}_n + \|\mathbf{v}_n\|^2\right] \\ &= \mathbb{E}\big[\|\mathbf{e}_n\|^2\big] + 2\mathbb{E}\big[\mathbf{e}_n \cdot \mathbf{u}_n\big] + 2\mathbb{E}\big[\mathbf{e}_n \cdot \mathbf{v}_n\big] + \mathbb{E}\big[\|\mathbf{u}_n\|^2\big] + 2\mathbb{E}\big[\mathbf{u}_n \cdot \mathbf{v}_n\big] + \mathbb{E}\big[\|\mathbf{v}_n\|^2\big] \end{aligned}$$

We can derive upper bounds for both $\mathbf{u}_n$ and $\mathbf{v}_n$ by Taylor expanding the exact solution and then using the Lipschitz continuity property of $\mathbf{a}(\mathbf{x})$ and $\mathbf{B}(\mathbf{x})$:

$$\mathbf{u}_n = \int_{t_n}^{t_n+\Delta t} (\mathbf{a}(\mathbf{x}(t)) - \mathbf{a}(\mathbf{x}_n))\, dt = \int_{t_n}^{t_n+\Delta t} \left(\nabla \mathbf{a}\Big|_{\mathbf{x}_n} [\mathbf{x}(t) - \mathbf{x}_n] + (\text{higher-order terms}) \right) dt$$

Express the term $\mathbf{x}(t) - \mathbf{x}_n$ in terms of error $\mathbf{e}_n$:

$$\mathbf{x}(t) - \mathbf{x}_n = \underbrace{(\mathbf{x}(t_n) - \mathbf{x}_n)}_{\mathbf{e}_n} + \int_{t_n}^{t} \mathbf{a}(\mathbf{x}(t))dt + \int_{t_n}^{t} \mathbf{B}(\mathbf{x}(t))d\mathbf{w}(t)$$

Substitute this expression for $\mathbf{x}(t) - \mathbf{x}_n$ into the term under the integral:

$$\mathbf{u}_n = \int_{t_n}^{t_n+\Delta t} \left(\nabla \mathbf{a}\Big|_{\mathbf{x}_n} \left[\mathbf{e}_n + \int_{t_n}^{t} \mathbf{a}(\mathbf{x}(t))dt + \int_{t_n}^{t} \mathbf{B}(\mathbf{x}(t))d\mathbf{w}(t) \right] + (\text{higher-order terms}) \right) dt$$

Since $\mathbf{e}_n = \mathbf{x}(t_n) - \mathbf{x}_n$ is time-independent and $\nabla \mathbf{a}\Big|_{\mathbf{x}_n}$ is bounded by the Lipschitz constant $L_{\mathbf{a}}$:

$$\mathbf{u}_n \leq L_{\mathbf{a}} \mathbf{e}_n \Delta t + \int_{t_n}^{t_n+\Delta t} \left(L_{\mathbf{a}} \left[\int_{t_n}^{t} \mathbf{a}(\mathbf{x}(t))dt + \int_{t_n}^{t} \mathbf{B}(\mathbf{x}(t))d\mathbf{w}(t) \right] + (\text{higher-order terms}) \right) dt$$

Performing the same steps for $\mathbf{v}_n$:

$$\mathbf{v}_n = \int_{t_n}^{t_n+\Delta t} (\mathbf{B}(\mathbf{x}(t)) - \mathbf{B}(\mathbf{x}_n)\, d\mathbf{w}(t) = \int_{t_n}^{t_n+\Delta t} \left(\nabla \mathbf{B}\Big|_{\mathbf{x}_n} [\mathbf{x}(t) - \mathbf{x}_n] + (\text{higher-order terms}) \right) d\mathbf{w}(t)$$

Substituting in the expression for $\mathbf{x}(t) - \mathbf{x}_n$:

$$\mathbf{v}_n = \int_{t_n}^{t_n+\Delta t} \left(\nabla \mathbf{B}\Big|_{\mathbf{x}_n} \left[\mathbf{e}_n + \int_{t_n}^{t} \mathbf{a}(\mathbf{x}(t))dt + \int_{t_n}^{t} \mathbf{B}(\mathbf{x}(t))d\mathbf{w}(t) \right] + (\text{higher-order terms}) \right) d\mathbf{w}(t)$$

Since $\mathbf{e}_n = \mathbf{x}(t_n) - \mathbf{x}_n$ is a constant and $\nabla \mathbf{B}\Big|_{\mathbf{x}_n}$ is bounded by the Lipschitz constant $L_{\mathbf{B}}$:

$$\mathbf{v}_n \leq L_{\mathbf{B}} \mathbf{e}_n (\mathbf{w}_{n+1} - \mathbf{w}_n) + \int_{t_n}^{t_n+\Delta t} \left(L_{\mathbf{B}} \left[\int_{t_n}^{t} \mathbf{a}(\mathbf{x}(t))dt + \int_{t_n}^{t} \mathbf{B}(\mathbf{x}(t))d\mathbf{w}(t) \right] + (\text{higher-order terms}) \right) d\mathbf{w}$$

Calculate each of the terms to determine the expected value of $\mathbb{E}\big[\|\mathbf{e}_{n+1}\|^2\big]$:

1. For $\mathbb{E}\big[\mathbf{e}_n \cdot \mathbf{u}_n\big]$:

$$\mathbb{E}\big[\mathbf{e}_n \cdot \mathbf{u}_n\big] \leq L_{\mathbf{a}}\mathbb{E}\left[\|\mathbf{e}_n\|^2\right] \Delta t + \text{(higher-order terms)}$$

2. For $\mathbb{E}\big[\mathbf{e}_n \cdot \mathbf{v}_n\big]$:

$$\mathbb{E}\big[\mathbf{e}_n \cdot \mathbf{v}_n\big] = \text{(higher-order terms)}$$

3. For $\mathbb{E}\big[\|\mathbf{u}_n\|^2\big]$:

$$\mathbb{E}\big[\|\mathbf{u}_n\|^2\big] \leq L_{\mathbf{a}}^2\mathbb{E}\left[\|\mathbf{e}_n\|^2\right] \Delta t^2 + \text{(higher-order terms)}$$

4. For $\mathbb{E}\big[\mathbf{u}_n \cdot \mathbf{v}_n\big]$:

$$\mathbb{E}\big[\mathbf{u}_n \cdot \mathbf{v}_n\big] = \text{(higher-order terms)}$$

5. For $\mathbb{E}\big[\|\mathbf{v}_n\|^2\big]$:

$$\mathbb{E}\big[\|\mathbf{v}_n\|^2\big] = L_{\mathbf{B}}^2\mathbb{E}\left[\|\mathbf{e}_n\|^2\right] \Delta t + \text{(higher-order terms)}$$

Putting everything together:

$$\begin{aligned}\mathbb{E}\left[\|\mathbf{e}_{n+1}\|^2\right] &\leq \mathbb{E}\left[\|\mathbf{e}_n\|^2\right] + L_{\mathbf{a}}\mathbb{E}\left[\|\mathbf{e}_n\|^2\right]\Delta t + L_{\mathbf{B}}^2\mathbb{E}\left[\|\mathbf{e}_n\|^2\right]\Delta t + \text{(higher-order terms)}\\ &\leq \big(1 + (L_{\mathbf{a}} + L_{\mathbf{B}}^2)\Delta t\big)\,\mathbb{E}\left[\|\mathbf{e}_n\|^2\right] + \text{(higher-order terms)}\end{aligned}$$

4.2.2 Weak Convergence Order

Let $\phi(\mathbf{x})$ an arbitrary but differentiable function. We try to estimate

$$|\mathbb{E}[\phi(\mathbf{x}(t_n))] - \mathbb{E}[\phi(\mathbf{x}_n)]|\,. \tag{81}$$

Writing $\langle\cdot\rangle$, substituting the exact solution from Equation 57 over a time interval $[t_n, t_n + \Delta t]$ and substituting the approximate solution from Equation 80, we get

$$|\langle\phi(\mathbf{x}(t_{n+1}))\rangle - \langle\phi(\mathbf{x}_{n+1})\rangle| = \left|\langle\phi(\mathbf{x}(t_n))\rangle + \int_{t_n}^{t_n+\Delta t}\left\langle\left(\frac{\partial\phi}{\partial t} + \nabla\phi\cdot\mathbf{a} + \frac{1}{2}\mathrm{Tr}\left(\mathbf{B}\mathbf{B}^T\nabla^2\phi\right)\right)\right\rangle dt - \langle\phi(\mathbf{x}_{n+1})\rangle\right|$$

Taylor expanding the term $\phi(\mathbf{x}_{n+1}))\rangle$ around $\mathbf{x}_n$:

$$\begin{aligned}\phi(\mathbf{x}_{n+1}) &= \phi(\mathbf{x}_n) + (\mathbf{x}_{n+1} - \mathbf{x}_n)^T\nabla\phi + \frac{1}{2}(\mathbf{x}_{n+1} - \mathbf{x}_n)^T\nabla^2\phi(\mathbf{x}_{n+1} - \mathbf{x}_n)\\ &\quad + \text{(higher-order terms)}\\ &= \phi(\mathbf{x}_n) + (\mathbf{a}(\mathbf{x}_n)\,\Delta t + \mathbf{B}(\mathbf{x}_n)\;(\mathbf{w}_{n+1} - \mathbf{w}_n))^T\nabla\phi\\ &\quad + \frac{1}{2}(\mathbf{a}(\mathbf{x}_n)\,\Delta t + \mathbf{B}(\mathbf{x}_n)\;(\mathbf{w}_{n+1} - \mathbf{w}_n))^T\nabla^2\phi(\mathbf{a}(\mathbf{x}_n)\,\Delta t\\ &\quad + \mathbf{B}(\mathbf{x}_n)\;(\mathbf{w}_{n+1} - \mathbf{w}_n)) + \text{(higher-order terms)}\end{aligned}$$

Taking expectations on both sides ($\Delta w_j^2 = \Delta t$) and Taylor expanding the term under the integral yields

$$|\langle\phi(\mathbf{x}(t_{n+1}))\rangle - \langle\phi(\mathbf{x}_{n+1})\rangle| \leq C\Delta t^2$$

Taking the worst case for every timestep, the total error is

$$C\Delta t^2 \frac{T}{\Delta t} = C'\Delta t$$

And thus

$$|\mathbb{E}[\phi(\mathbf{x}(t_n))] - \mathbb{E}[\phi(\mathbf{x}_n)]| \leq C'\Delta t \tag{82}$$

4.2.3 Implementation

Implementation of the forward Euler method (see Equation 80): Discretize time into N_t time steps. Solve the equation for N_s ensemble realizations. In summary: important measures:

- N_t: Number of time steps $T/\Delta t$
- N_s: Number of Monte Carlo steps (ensemble realizations)
- N: Number of state dimensions (state vector $\mathbf{x}$)
- M: Number of noise (Wiener process $\mathbf{w}$) dimensions

For more efficient looping: pre-allocate Wiener process increments $\Delta\mathbf{w}_n$ for all MC steps for all time steps:

$$\underbrace{\left[\mathrm{M} \left\{ \overbrace{\begin{pmatrix} \Delta\mathbf{w}_1^{(1)} & \cdots & \Delta\mathbf{w}_1^{(N_\mathrm{s})} \end{pmatrix}}^{N_\mathrm{s}}, \quad \cdots \quad \begin{pmatrix} \Delta\mathbf{w}_{N_\mathrm{t}}^{(1)} & \cdots & \Delta\mathbf{w}_{N_\mathrm{t}}^{(N_\mathrm{s})} \end{pmatrix} \right.\right]}_{N_\mathrm{t} \text{ matrices}} \tag{83}$$

Vectorize updating the solution:

$$\mathbf{X}_n = \left.\underbrace{\left[\mathbf{x}_n^{(1)} \cdots \mathbf{x}_n^{(N_\mathrm{s})}\right]}_{N_\mathrm{s}}\right\} N \tag{84}$$

$$\mathbf{A}(\mathbf{X}_n) = \left.\underbrace{\left[\mathbf{a}(\mathbf{x}_n^{(1)}) \cdots \mathbf{a}(\mathbf{x}_n^{(N_\mathrm{s})})\right]}_{N_\mathrm{s}}\right\} N \tag{85}$$

Less expensive to loop over state dimensions N than MC steps

$$\mathbf{B}(\mathbf{X}_n) = \underbrace{\left[N_\mathrm{s} \left\{ \overbrace{\begin{pmatrix} \mathbf{B}_{11}(\mathbf{x}_n^{(1)}) & \cdots & \mathbf{B}_{1M}(\mathbf{x}_n^{(1)}) \\ \vdots & & \vdots \\ \mathbf{B}_{11}(\mathbf{x}_n^{(N_\mathrm{s})}) & \cdots & \mathbf{B}_{1M}(\mathbf{x}_n^{(N_\mathrm{s})}) \end{pmatrix}}^{M}, \quad \cdots \quad \begin{pmatrix} \mathbf{B}_{N1}(\mathbf{x}_n^{(1)}) & \cdots & \mathbf{B}_{NM}(\mathbf{x}_n^{(1)}) \\ \vdots & & \vdots \\ \mathbf{B}_{N1}(\mathbf{x}_n^{(N_\mathrm{s})}) & \cdots & \mathbf{B}_{NM}(\mathbf{x}_n^{(N_\mathrm{s})}) \end{pmatrix} \right.\right]}_{N \text{ matrices}} \tag{86}$$

4.3 Milstein's Method

Since the convergence order-limiting term is the diffusion integral, Milstein's method aims for a more accurate approximation by including higher order terms. Using Ito's Lemma, expand $B_{ij}(\mathbf{x}(t))$ around $(\mathbf{x}_n)$ up to 1st order:

$$\begin{aligned} B_{ij}(\mathbf{x}(t)) \approx B_{ij}(\mathbf{x}_n) + \frac{\partial B_{ij}(\mathbf{x})}{\partial t}\Big|_{\mathbf{x}_n}(t-t_n) \\ + \sum_{k=1}^{N} \frac{\partial B_{ij}(\mathbf{x})}{\partial x_k}\Big|_{\mathbf{x}_n}(x_k(t) - x_k(t_n)) + (\text{higher order terms}) \end{aligned} \tag{87}$$

Substituting this expression into the integral in Equation 73 yields:

$$\begin{aligned} \int_{t_n}^{t_n+\Delta t} B_{ij}(\mathbf{x}) dw_j(t) \approx B_{ij}(\mathbf{x}_n) \int_{t_n}^{t_n+\Delta t} dw_j(t) \\ + \sum_{k=1}^{N} \frac{\partial B_{ij}(\mathbf{x})}{\partial x_k}\Big|_{\mathbf{x}_n} \int_{t_n}^{t_n+\Delta t} (x_k(t) - x_k(t_n)) dw_j(t) \\ + \frac{\partial B_{ij}(\mathbf{x})}{\partial t}\Big|_{\mathbf{x}_n} \int_{t_n}^{t_n+\Delta t} (t-t_n) dw_j(t) \end{aligned} \tag{88}$$

Approximate the term $x_k(t)$ under the integral via a 0-th order expansion of the drift term $a_k(\mathbf{x}(t)) \approx a_k(\mathbf{x}(t_n))$:

$$x_k(t) \approx x_k(t_n) + a_k(\mathbf{x}(t_n))(t-t_n) + \sum_{l=1}^{M} \int_{t_n}^{t} B_{kl}(\mathbf{x}(t)) dw_l(t) \tag{89}$$

Substituting this expression into the 1st order expansion of the integral above yields:

$$\begin{aligned} \int_{t_n}^{t_n+\Delta t} B_{ij}(\mathbf{x}) dw_j(t) \approx\ & B_{ij}(\mathbf{x}_n) \int_{t_n}^{t_n+\Delta t} dw_j(t) + \frac{\partial B_{ij}(\mathbf{x})}{\partial t}\Big|_{\mathbf{x}_n} \int_{t_n}^{t_n+\Delta t} (t-t_n) dw_j(t) \\ + \sum_{k=1}^{N} \frac{\partial B_{ij}(\mathbf{x})}{\partial x_k}\Big|_{\mathbf{x}_n} & \int_{t_n}^{t_n+\Delta t} \left(\left[x_k(t_n) + a_k(\mathbf{x}(t_n))(t-t_n) + \sum_{l=1}^{M} \int_{t_n}^{t} B_{kl}(\mathbf{x}(t)) dw_l(t) \right] - x_k(t_n) \right) dw_j(t) \end{aligned}$$

We only include terms up to $O(\Delta t)$; any term involving tdw is of order $O(\Delta t^{1.5})$:

$$\begin{aligned} \int_{t_n}^{t_n+\Delta t} B_{ij}(\mathbf{x}) dw_j(t) \approx\ & B_{ij}(\mathbf{x}_n)(w_j(t_{n+1}) - w_j(t_n)) \\ + \sum_{k=1}^{N} \frac{\partial B_{ij}(\mathbf{x})}{\partial x_k}\Big|_{\mathbf{x}_n} & \int_{t_n}^{t_n+\Delta t} \left(\left[\sum_{l=1}^{M} \int_{t_n}^{t} B_{kl}(\mathbf{x}(t)) dw_l(t) \right] \right) dw_j(t) \end{aligned}$$

Approximate $B_{kl}(\mathbf{x}(t)) \approx B_{kl}(\mathbf{x}(t_n))$ under the integral:

$$\begin{aligned} \int_{t_n}^{t_n+\Delta t} B_{ij}(\mathbf{x}) dw_j(t) \approx\ & B_{ij}(\mathbf{x}_n)(w_j(t_{n+1}) - w_j(t_n)) \\ + \sum_{k=1}^{N} \sum_{l=1}^{M} \frac{\partial B_{ij}(\mathbf{x})}{\partial x_k} B_{kl}(\mathbf{x})\Big|_{\mathbf{x}_n} & \int_{t_n}^{t_n+\Delta t} \int_{t_n}^{t} dw_l(t) dw_j(t) + (\text{higher-order terms}) \end{aligned}$$

The last integral can be solved using Ito's Lemma (for more information, google it):

$$\int_{t_n}^{t_n+\Delta t}\int_{t_n}^{t} dw_l(t)dw_j(t) = \begin{cases} \text{if } l = j & \frac{1}{2}\left((w_j(t_{n+1}) - w_j(t_n))^2 - \Delta t\right) \\ \text{if } l \neq j & 0 \end{cases}$$

Substituting this term into the diffusion integral and then substituting the expression for this integral into the original scheme, we obtain the Milstein method:

$$\begin{aligned} x_i^{n+1} &= x_i^n + a_i(\mathbf{x}_n)\,\Delta t + \sum_{j=1}^{M} B_{ij}(\mathbf{x}_n)\left(w_j^{n+1} - w_j^n\right) \\ &+ \frac{1}{2}\sum_{k=1}^{N}\frac{\partial B_{ij}^n}{\partial x_k}B_{kj}^n\left((w_j^{n+1} - w_j^n)^2 - \Delta t\right) \end{aligned} \tag{90}$$

5 Minimal Examples

5.1 Pure Diffusion

Consider a one-dimensional system with initial state x_0. The time evolution is governed by an overdamped Langevin equation (see subsection 1.8 with no drift ($\mathbf{a}(\mathbf{x}, t) = 0$) and isotropic diffusion ($\mathbf{B}(\mathbf{x}, t) = B$)

$$\dot{x} = B\xi(t). \tag{91}$$

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

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

$$\begin{aligned} \dot{x}(t) &= B\xi(t) \\ x(t) &= B\int_0^t \xi(t')\,dt' \\ \langle x(t) \rangle &= B\int_0^t \langle \xi(t') \rangle\,dt' = B\int_0^t 0\,dt' = 0 \end{aligned} \tag{92}$$

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

$$\begin{aligned} x^2(t) &= \left(B\int_0^t \xi(t')\,dt'\right)^2 = B^2\int_0^t\int_0^t \xi(t')\xi(t'')\,dt'dt'' \\ \left\langle x^2(t) \right\rangle &= \left\langle B^2\int_0^t\int_0^t \xi(t')\xi(t'')\,dt'dt'' \right\rangle = B^2\int_0^t\int_0^t \langle \xi(t')\xi(t'') \rangle\,dt'\,dt'' \\ &= B^2\int_0^t\int_0^t \delta(t''-t')\,dt'\,dt'' = B^2\int_0^t dt'' = B^2 t \end{aligned} \tag{93}$$

The variance is then

$$\langle\langle x(t) \rangle\rangle = \left\langle x^2(t) \right\rangle - \langle x(t) \rangle^2 = B^2 t - 0 = B^2 t \tag{94}$$

5.1.2 Computing Mean and Variance via Ito's Lemma

Ito's Lemma (see subsection 1.7), applied to a function $f(x)$ for this system is

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

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

$$\begin{aligned} \langle dx \rangle = 0 \quad &\rightarrow \quad \langle x(t) \rangle = x_0 \\ \left\langle dx^2 \right\rangle = B^2\,dt \quad &\rightarrow \quad \left\langle x^2(t) \right\rangle = x_0^2 + B^2 t \\ &\rightarrow \quad \langle\langle x(t) \rangle\rangle = \left\langle x^2(t) \right\rangle - \langle x(t) \rangle^2 = B^2 t \end{aligned}$$

5.1.3 Computing Mean and Variance via the Fokker-Planck Equation

The Fokker-Planck equation for this system reads

$$\begin{aligned}\frac{\partial p(x,t)}{\partial t} &= \frac{1}{2}B^2\frac{\partial^2 p}{\partial x^2}\\ p(x,0) &= \delta(x-x_0)\end{aligned}$$

which is a linear parabolic PDE. Solution:

1. Transform in Fourier space:

$$\begin{aligned}\hat{p}(\omega,t) &= \int_{-\infty}^{\infty} p(x,t)e^{-i\omega x}\,dx\\ \hat{p}(\omega,0) &= e^{-i\omega x_0}\end{aligned}$$

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

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

3. Inverse Fourier transform back into state space

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

4. perform quadratic completion

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

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

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

5. Solve integral with error function

$$\begin{aligned}\int_{-\infty}^{\infty} e^{-az^2}dz &= \sqrt{\frac{\pi}{a}}\\ \int_{-\infty}^{\infty} e^{-\frac{B^2t}{2}\left(\omega-\frac{i(x-x_0)}{B^2t}\right)^2}d\omega &= \sqrt{\frac{2\pi}{B^2t}} \quad \text{with } a = \frac{B^2t}{2}\end{aligned}$$

6. Final solution:

$$p(x,t) = \frac{1}{\sqrt{2\pi B^2t}}e^{-\frac{(x-x_0)^2}{2B^2t}} \tag{95}$$

This is the PDF of a Gaussian distribution with

$$\boxed{\begin{aligned}\langle x(t)\rangle &= x_0 && (96)\\ \langle\langle x(t)\rangle\rangle &= \langle x^2(t)\rangle - \langle x(t)\rangle^2 = B^2t && (97)\end{aligned}}$$

5.1.4 Numerical Solution

Convert the SDE into a dimensionless SDE: Introduce a change of variables $\hat{t} = t/t_0$ and $\hat{x} = x/x_0$. Substitute into the old equation:

$$\dot{x}(\hat{t}) = \frac{\mathrm{d}(x_0\hat{x})}{\mathrm{d}\hat{t}}\frac{\mathrm{d}\hat{t}}{\mathrm{d}t} = \frac{x_0}{t_0}\frac{\mathrm{d}\hat{x}}{\mathrm{d}\hat{t}} = B\frac{\xi(\hat{t})}{\sqrt{t_0}} \tag{98}$$

Let $x_0 = B\sqrt{t_0}$. The dimensionless SDE then becomes

$$\dot{\hat{x}}(\hat{t}) = \xi(\hat{t}) \tag{99}$$

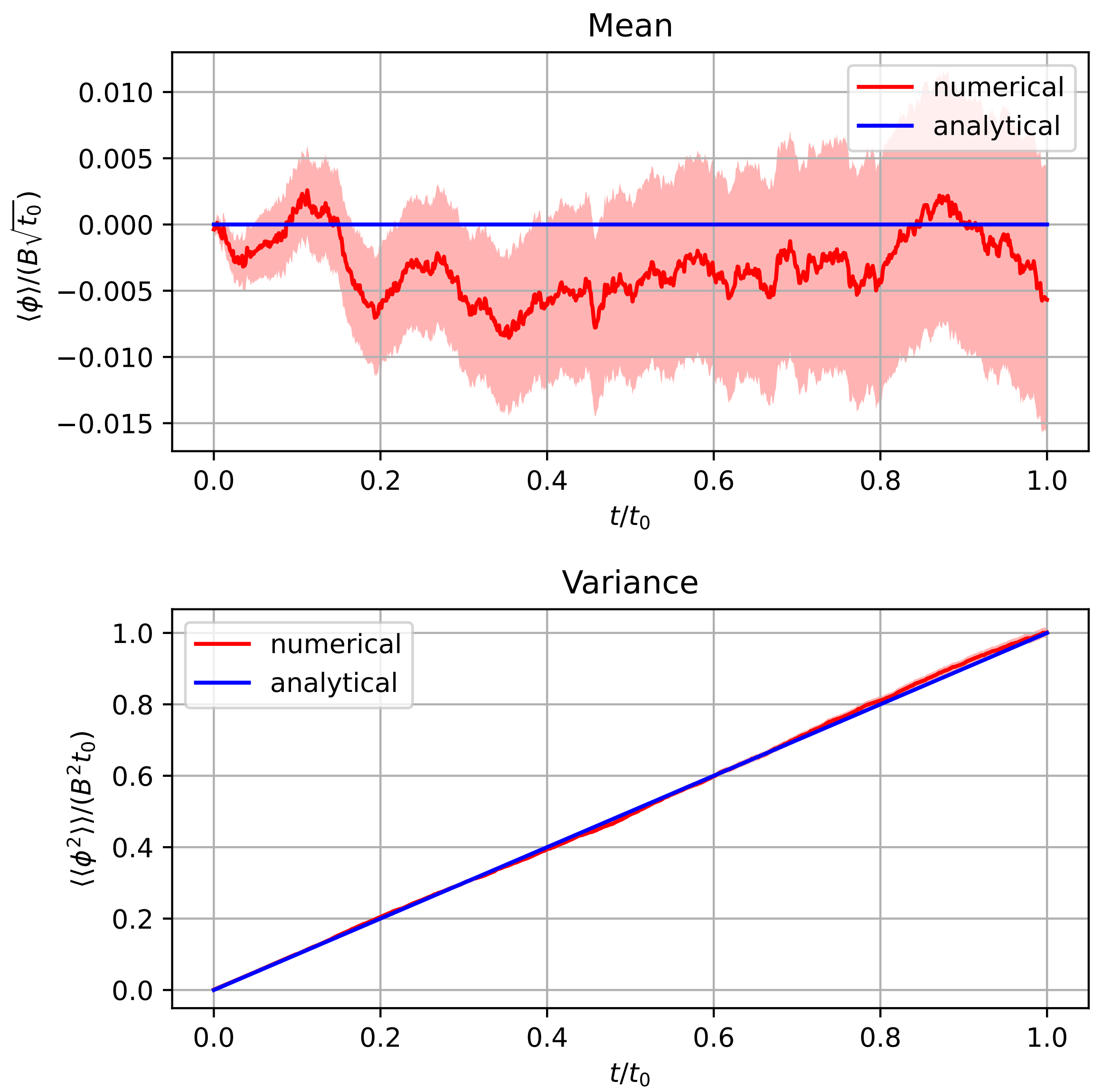

Figure 1: $\hat{T} = 1$, $N_\mathrm{t} = 10^4$ time steps. $N_\mathrm{s} = 10^4$ MC-steps (ensemble-realizations). The shaded region corresponds to the 1σ-interval

5.2 LR Circuit with Current Source

Consider an electrical circuit consisting of

- Ohmic Resistor:
$$\dot{\phi}_{\rm R} = RI_{\rm R} = U_{\rm R} \tag{100}$$
- Coil:
$$\dot{\phi}_{\rm L} = L\frac{{\rm d}I_{\rm L}}{{\rm d}t} = U_{\rm L} \quad \rightarrow \quad \phi_{\rm L} = LI_{\rm L} \tag{101}$$
- Current Source I_0

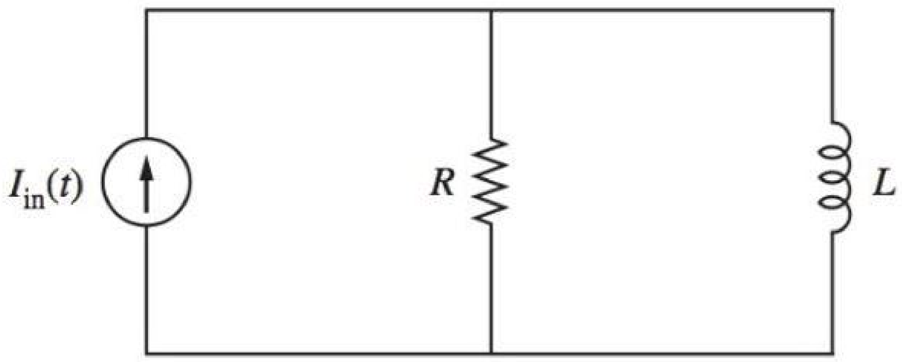

Figure 2: LR Circuit

Kirchhoff's rules yield:

$$U_{\rm R} = U_{\rm L} \tag{102}$$
$$I_{\rm R} + I_{\rm L} = I_0 \tag{103}$$

Substituting node flux for current and voltage results in

$$I_{\rm R} + I_{\rm L} = \frac{\dot{\phi}_{\rm R}}{R} + \frac{\phi_{\rm L}}{L} = I_0 \tag{104}$$

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

$$\frac{\dot{\phi}}{R} + \frac{\phi}{L} = I_0 \tag{105}$$

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

$$\dot{\phi} = -\frac{R}{L}\phi + B\xi(t). \tag{106}$$

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

5.2.1 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 61) to obtain the consistent diffusion term B: With

$$\langle A(x,t))x\rangle = -\left\langle \frac{R}{L}\phi^2 \right\rangle = -2R\left\langle \frac{\phi^2}{2L} \right\rangle = -R\, H_\mathrm{L} = -R\left\langle \phi \frac{\mathrm{d}}{\mathrm{d}\phi}\frac{\phi^2}{2L} \right\rangle = -R\left\langle \phi \frac{\mathrm{d}}{\mathrm{d}\phi} H_\mathrm{L} \right\rangle \tag{107}$$

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

$$\langle A(x,t))x\rangle = -\frac{R}{\beta} \tag{108}$$

and then using the Fluctuation-Dissipation theorem (see subsection 1.11), we obtain

$$B = \sqrt{-2\,\langle A(,t))x_k\rangle} = \sqrt{2Rk_\mathrm{B}T} \tag{109}$$

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

5.2.2 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

$$\phi(t) = \phi(0)e^{-\frac{R}{L}t} + B\int_0^t e^{-\frac{R}{L}(t-\tau)}\xi(\tau)\, d\tau \tag{110}$$

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,

$$\begin{aligned}\langle \phi(t)\rangle &= \left\langle \phi(0)e^{-\frac{R}{L}t} \right\rangle + B\int_0^t e^{-\frac{R}{L}(t-\tau)}\,\langle \xi(\tau)\rangle\, d\tau = \\ &= \phi(0)e^{-\frac{R}{L}t}\end{aligned} \tag{111}$$

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

$$\begin{aligned}\left\langle \phi^2(t)\right\rangle &= \left\langle \phi^2(0)e^{-\frac{2R}{L}t}\right\rangle + B^2\int_0^t\int_0^t e^{-\frac{R}{L}(t-\tau)}e^{-\frac{R}{L}(t-\tau')}\left\langle \xi(\tau)\xi(\tau')\right\rangle\, d\tau d\tau' \\ &= \phi^2(0)e^{-\frac{2R}{L}t} + B^2\int_0^t\int_0^t e^{-\frac{R}{L}(t-\tau)}e^{-\frac{R}{L}(t-\tau')}\delta(\tau-\tau')\, d\tau d\tau' \\ &= \phi^2(0)e^{-\frac{2R}{L}t} + B^2\int_0^t e^{-\frac{2R}{L}(t-\tau)}\, d\tau \\ &= \phi^2(0)e^{-\frac{2R}{L}t} + \frac{B^2L}{2R}\left(1-e^{-\frac{2R}{L}t}\right) \end{aligned} \tag{112}$$

The variance is then

$$\begin{aligned}\langle\langle\phi(t)\rangle\rangle &= \left\langle\phi^2(t)\right\rangle - \langle\phi(t)\rangle^2 = \phi^2(0)e^{-\frac{2R}{L}t} + \frac{B^2L}{2R}\left(1-e^{-\frac{2R}{L}t}\right) - \phi^2(0)e^{-\frac{2R}{L}t} \\ &= \frac{B^2L}{2R}\left(1-e^{-\frac{2R}{L}t}\right) = k_{\mathrm{B}}TL\left(1-e^{-\frac{2R}{L}t}\right)\end{aligned} \tag{113}$$

In summary:

$$\boxed{\begin{aligned}\langle\phi(t)\rangle &= \phi(0)e^{-\frac{R}{L}t} && (114)\\ \langle\langle\phi^2(t)\rangle\rangle &= k_{\mathrm{B}}TL\left(1-e^{-\frac{2R}{L}t}\right) && (115)\end{aligned}}$$

5.2.3 Computing Mean and Variance via the Fokker-Planck Equation

The Fokker-Planck equation for this system reads

$$\frac{\partial p(\phi,t)}{\partial t} = \frac{R}{L}\frac{\partial}{\partial p}(\phi p) + \frac{1}{2}B^2\frac{\partial^2 p}{\partial\phi^2} \tag{116}$$

$$p(\phi,0) = \delta(\phi-\phi(0)) \tag{117}$$

Linear parabolic PDE: Solve using Fourier Transform

1. Transform in Fourier space:

$$\hat{p}(\omega,t) = \int_{-\infty}^{\infty} p(\phi,t)e^{-i\omega\phi}\, d\phi \tag{118}$$

$$\hat{p}(\omega,0) = e^{-i\omega x_0} \tag{119}$$

2. In Fourier space, the PDE reads:

$$\frac{\partial\tilde{p}}{\partial t} = \frac{R}{L}\left(-i\frac{\partial}{\partial\omega}(\omega\tilde{p}) + \tilde{p}\right) - \frac{1}{2}B^2\omega^2\tilde{p} \tag{120}$$

3. Ansatz:

$$\tilde{p}(\omega,t) = e^{f(\omega,t)} \tag{121}$$

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

$$f(\omega,t) = -i\omega\phi(0)e^{-\frac{R}{L}t} - \frac{B^2L}{4R}\omega^2\left(1-e^{-\frac{2R}{L}t}\right) \tag{122}$$

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

$$\mu(t) = \phi(0)e^{-\frac{R}{L}t} \tag{123}$$

$$\sigma^2(t) = \frac{B^2L}{2R}\left(1-e^{-\frac{2R}{L}t}\right) \tag{124}$$

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

5.2.4 Numerical Solution

Convert the SDE into a dimensionless SDE: Introduce a change of variables $\hat{t} = t/t_0$ and $\varphi = \phi/\phi_0$. Substitute into the old equation:

$$\dot{\phi}(\hat{t}) = \frac{\mathrm{d}(\phi_0\varphi(\hat{t}))}{\mathrm{d}\hat{t}}\frac{\mathrm{d}\hat{t}}{\mathrm{d}t} = \frac{\phi_0}{t_0}\frac{\mathrm{d}\varphi(\hat{t})}{\mathrm{d}\hat{t}} = -\frac{R}{L}\varphi(\hat{t})\phi_0 + \sqrt{2Rk_\mathrm{B}T}\frac{\xi(\hat{t})}{\sqrt{t_0}} \tag{125}$$

Rearranging, where $\dot{(\cdot)}$ now denotes $d/d\hat{t}$:

$$\dot{\varphi}(\hat{t}) = -t_0\frac{R}{L}\varphi(\hat{t}) + \frac{\sqrt{t_0}}{\phi_0}\sqrt{2Rk_\mathrm{B}T}\xi(\hat{t}) \tag{126}$$

Take the reference time and reference node flux $t_0 = L/R$ and $\phi_0 = \sqrt{2k_\mathrm{B}TL}$. The SDE then becomes

$$\dot{\varphi}(\hat{t}) = -\varphi(\hat{t}) + \xi(\hat{t}) \tag{127}$$

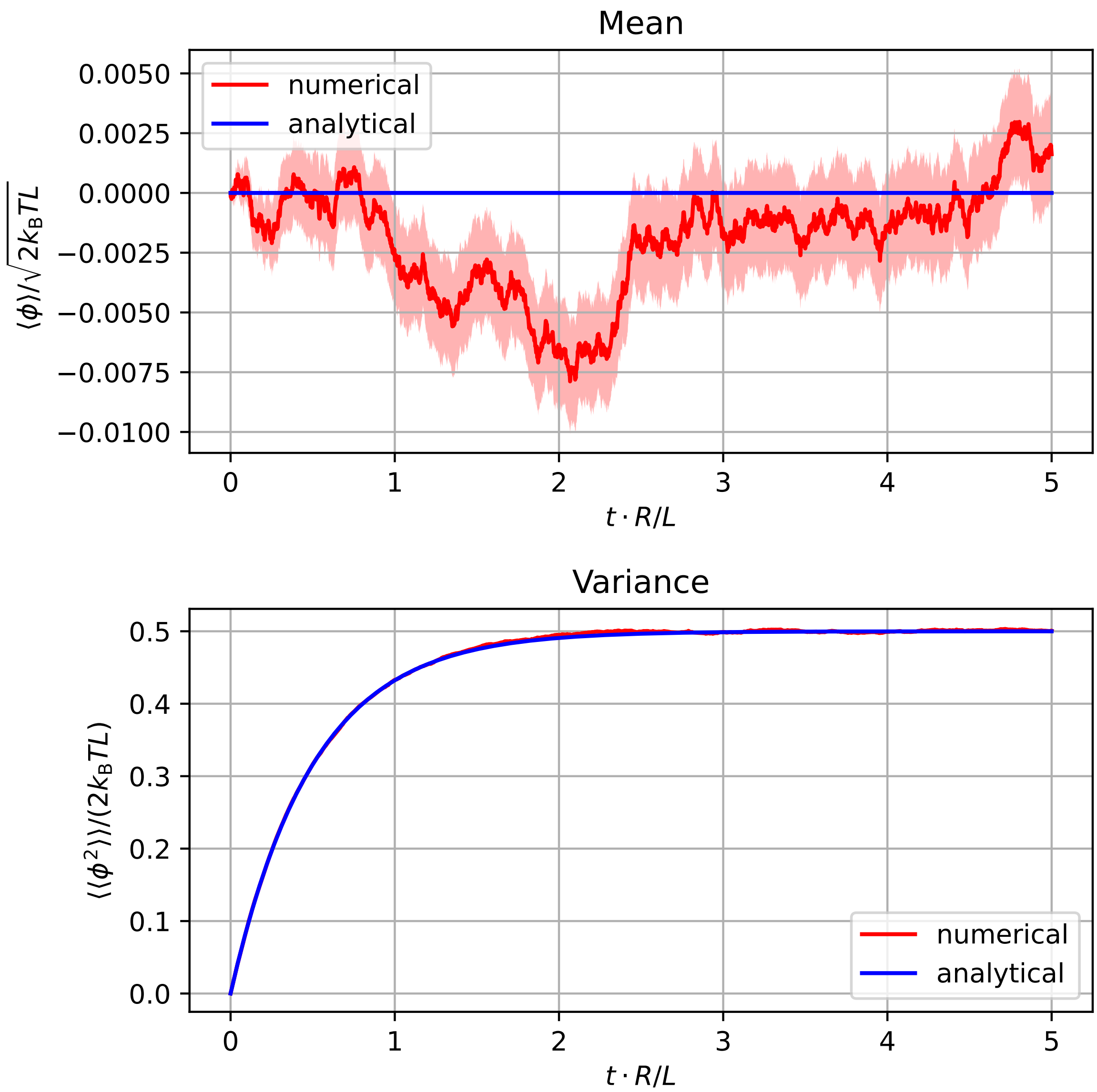

Figure 3: $\hat{T} = 5$, $N_{\mathrm{t}} = 10^5$ time steps. $N_{\mathrm{s}} = 5 \cdot 10^3$ MC-steps (ensemble-realizations). The shaded region corresponds to the 1σ-interval

5.3 Resistor with Current Source

Consider an electrical circuit consisting of

- Ohmic Resistor:
$$\dot{\phi}_{\mathrm{R}} = RI_{\mathrm{R}} = U_{\mathrm{R}} \tag{128}$$

- Current Source I_0

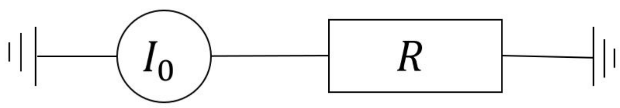

Figure 4: Resistor circuit

By using Kirchhoff's rules, we obtain the ODE

$$I_{\mathrm{R}} = \frac{U_{\mathrm{R}}}{R} = \frac{\dot{\phi}_{\mathrm{R}}}{R} = I_0. \tag{129}$$

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 1.8)

$$\dot{\phi}_{\mathrm{R}} = RI_0 + B\xi(t) \tag{130}$$

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 109). Per convention, instead we use the notation $B = \alpha/R$ with $\alpha = \sqrt{2k_{\mathrm{B}}T/R}$, which yields the SDE

$$\dot{\phi}_{\mathrm{R}} = RI_0 + \frac{\alpha}{R}\xi(t) \tag{131}$$

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

Integrating both sides with respect to time yields

$$\phi(t) = \int_0^t (RI_0 + \frac{\alpha}{R}\xi(t'))\, dt' \tag{132}$$

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

$$\langle \phi(t) \rangle = \int_0^t (RI_0 + \frac{\alpha}{R}\langle \xi(t') \rangle\, dt' = RI_0 t$$

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

$$\begin{aligned}
\langle \phi^2(t) \rangle &= \left\langle \left(\int_0^t (RI_0 + \frac{\alpha}{R}\xi(t'))\, dt' \right)^2 \right\rangle \\
&= \int_0^t \int_0^t (R^2 I_0^2 + 2\frac{\alpha}{R}\langle \xi(t') \rangle + \left(\frac{\alpha}{R}\right)^2 \langle \xi(t')\xi(t'') \rangle \, dt' dt'' \\
&= (RI_0 t)^2 + \left(\frac{\alpha}{R}\right)^2 t = (RI_0 t)^2 + 2Rk_\mathrm{B}Tt
\end{aligned}$$

This yields the mean and variance

$$\boxed{\begin{aligned} \langle \phi(t) \rangle &= RI_0 t \qquad (133) \\ \langle\langle \phi^2(t) \rangle\rangle &= 2Rk_\mathrm{B}Tt \qquad (134) \end{aligned}}$$

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

5.3.2 The node flux obeys the TUR

The average entropy production σ of this system is

$$\sigma = \frac{1}{t} \int_0^t \left\langle \frac{Q}{T} \right\rangle dt' = \frac{1}{t} \int_0^t \frac{RI_0^2}{T} dt' = \frac{RI_0^2}{T}$$

Substituting into the TUR yields

$$\frac{\langle\langle \phi^2(t) \rangle\rangle}{\langle \phi(t) \rangle^2} \cdot \sigma t = \frac{2Rk_\mathrm{B}Tt}{R^2 I_0^2 t^2} \cdot \frac{RI_0^2}{T} t = 2k_\mathrm{B} \geq 2k_\mathrm{B} \tag{135}$$

which saturates the TUR.

5.3.3 Numerical Solution

Convert the SDE into a dimensionless SDE: Introduce a change of variables $\hat{t} = t/t_0$ and $\varphi = \phi/\phi_0$. Substitute into the original equation:

$$\dot{\phi}(\hat{t}) = \frac{\mathrm{d}(\phi_0 \varphi(\hat{t}))}{\mathrm{d}\hat{t}} \frac{\mathrm{d}\hat{t}}{\mathrm{d}t} = \frac{\phi_0}{t_0} \frac{\mathrm{d}\varphi(\hat{t})}{\mathrm{d}\hat{t}} = RI_0 + \sqrt{2Rk_\mathrm{B}T} \frac{\xi(\hat{t})}{\sqrt{t_0}} \tag{136}$$

Rearranging, where $\dot{(\cdot)}$ now denotes $d/d\hat{t}$:

$$\dot{\varphi}(\hat{t}) = \frac{t_0}{\phi_0} RI_0 + \frac{\sqrt{t_0}}{\phi_0} \sqrt{2Rk_\mathrm{B}T} \xi(\hat{t}) \tag{137}$$

Take the reference time and reference node flux $t_0 = 2k_\mathrm{B}T/(RI_0^2)$ and $\phi_0 = 2k_\mathrm{B}T/I_0$, the SDE becomes

$$\dot{\varphi}(\hat{t}) = 1 + \xi(\hat{t}) \tag{138}$$

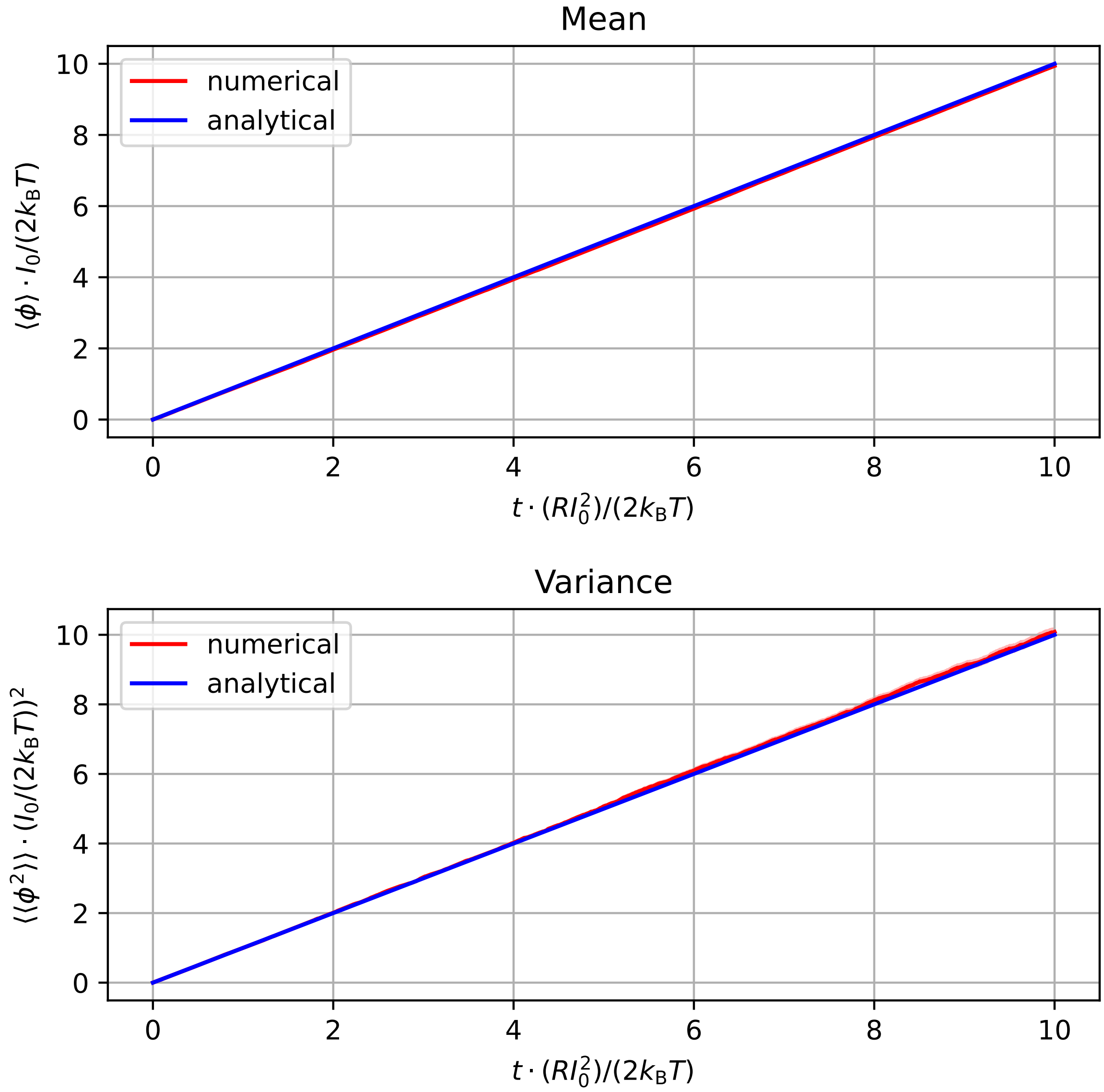

Figure 5: $\hat{T} = 1$, $N_\mathrm{t} = 10^4$ time steps. $N_\mathrm{s} = 10^4$ MC-steps (ensemble-realizations). The shaded region corresponds to the 1σ-interval

5.4 JJ-R Circuit

Consider a circuit made up of

- Ohmic Resistor

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

- Josephson Junction

$$I = I_{\mathrm{c}} \sin\left(\frac{2e}{\hbar}\phi\right)$$
$$\dot{\phi} = V$$

- Current source I_0

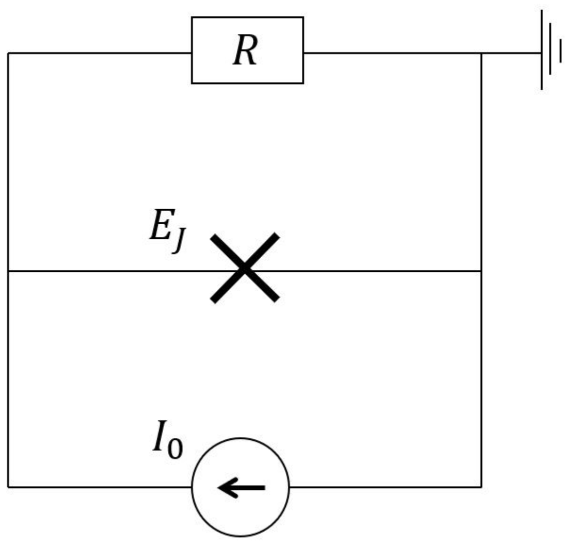

Figure 6: Circuit consisting of a Josephson junction and an ohmic resistor

Using Kirchhoff's rules, the sum of the current over the Josephson junction and the resistor must be equal to I_0. The voltage (and thus the node flux) over the resistor and the JJ are equal. The SDE for the circuit is

$$I_0 + \sqrt{\frac{2k_{\mathrm{B}}T}{R}}\xi(t) = \frac{\dot{\phi}}{R} + I_{\mathrm{c}} \sin\left(\frac{2e}{\hbar}\phi\right)$$

Rearranging:

$$\dot{\phi} = RI_0 - RI_{\mathrm{c}} \sin\left(\frac{2e}{\hbar}\phi\right) + \sqrt{2Rk_{\mathrm{B}}T}\xi(t)$$

Introduce a change of variables $\hat{t} = t/t_0$ and $\varphi = \phi/\phi_0$. Substitute into the original equation:

$$\dot{\phi}(t) = \frac{\mathrm{d}(\phi_0\varphi(\hat{t}))}{\mathrm{d}\hat{t}}\frac{\mathrm{d}\hat{t}}{\mathrm{d}t} = \frac{\phi_0}{t_0}\frac{\mathrm{d}\varphi(\hat{t})}{\mathrm{d}\hat{t}} = RI_0 - RI_{\mathrm{c}} \sin\left(\frac{2e}{\hbar}\phi_0\varphi(\hat{t})\right) + \sqrt{2Rk_{\mathrm{B}}T}\frac{\xi(\hat{t})}{\sqrt{t_0}}$$

Rearranging, where $\dot{(\cdot)}$ now denotes $d/d\hat{t}$:

$$\dot{\varphi}(\hat{t}) = \frac{t_0}{\phi_0} R I_0 - \frac{t_0}{\phi_0} R I_{\mathrm{c}} \sin\left(\frac{2e}{\hbar}\phi_0 \varphi(\hat{t})\right) + \frac{\sqrt{t_0}}{\phi_0}\sqrt{2Rk_{\mathrm{B}}T}\xi(\hat{t})$$

Choosing $\phi_0 = \hbar/(2e)$ and $t_0 = \hbar/(2eRI_{\mathrm{c}})$ and abbreviating $I_0/I_{\mathrm{c}} =: i$ leads to the dimensionless SDE

$$\boxed{\dot{\varphi}(\hat{t}) = i - \sin\left(\varphi(\hat{t})\right) + \sqrt{\frac{4ek_{\mathrm{B}}T}{\hbar I_{\mathrm{c}}}}\xi(\hat{t})} \tag{139}$$

5.4.1 Deterministic Solution

The dimensionless ODE without noise reads

$$\dot{\varphi}(\hat{t}) = i - \sin\left(\varphi(\hat{t})\right). \tag{140}$$

Using separation of variables ($i > 1$):

$$\int_{\varphi(0)}^{\varphi(t)} \frac{1}{i - \sin(\varphi)} d\varphi = \int_0^{\hat{t}} dt'$$

Choose $\varphi(0) = 0$. This integral has the standard solution

$$\frac{2}{\sqrt{i^2-1}} \arctan\left(\frac{-1 + i\tan(\varphi/2)}{\sqrt{i^2-1}}\right) = \hat{t}$$

Rearranging:

$$\boxed{\varphi(\hat{t}) = 2\arctan\left(\sqrt{1 - \frac{1}{i^2}}\tan\left(\frac{\hat{t}\sqrt{i^2-1}}{2}\right) + \frac{1}{i}\right)} \tag{141}$$

This function is periodic with period $\hat{T} = 2\pi/\sqrt{i^2-1}$ (since tan is $\pi-$periodic). Note however that $\varphi(\hat{t})$ itself is not $\pi-$periodic and ever-increasing. The difference $\varphi(\hat{t}+\hat{T}) - \varphi(\hat{t}) = \text{const} \neq 0$.

5.4.2 I-V Curve

The time-averaged voltage $\overline{V}$ is

$$\begin{aligned}\overline{V} = \frac{1}{T}\int_{-T/2}^{T/2} V(t)dt = \frac{1}{T}(\phi(T/2) - \phi(-T/2)) = \frac{\phi_0}{\hat{T}t_0}(\varphi(\hat{T}/2) - \varphi(-\hat{T}/2)) = \frac{2\pi\phi_0}{\hat{T}t_0} \\ = 2\pi\frac{\hbar}{2e}\frac{2eRI_{\mathrm{c}}}{\hbar}\frac{\sqrt{i^2-1}}{2\pi} = RI_{\mathrm{c}}\sqrt{i^2-1}\end{aligned}$$

When $i \to 1$ it follows that $\hat{T} \to \infty$. This yields $\varphi(\hat{t}) = \text{const} = \arcsin(i)$ and thus $\overline{V} = 0$ for $i \leq 1$.
In summary:

$$\boxed{\frac{\overline{V}(i)}{RI_{\mathrm{c}}} = \begin{cases} i > 1 & \sqrt{i^2-1} \\ i \leq 1 & 0 \end{cases}} \tag{142}$$

A References

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