

RWTH UNIVERSITY

INSTITUT FÜR QUANTENINFORMATION

# BA Notes

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# 1 Theorems

## 1.1 Equipartition Theorem

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

$$\frac{d\mathbf{q}}{dt} = \frac{\partial H}{\partial \mathbf{p}}, \quad (1)$$

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{q}}. \quad (2)$$

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 probabilities then sum to 1:

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

with the inverse temperature  $\beta = 1/(k_B T)$  and the infinitesimal volume

$$d\Gamma = \prod_i dp_i dq_i. \quad (4)$$

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

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

Using partial integration on [Equation 3](#), we obtain

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

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:

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

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

Rearranging yields

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

This result is called the Equipartition theorem. For a quadratic Hamiltonian, this expression simplifies to  $\langle H \rangle = k_B T/2$ .

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:

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

## 1.2 Divergence Theorem - Partial Integration

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

$$\int_{\Omega} \nabla \cdot (\mathbf{f}p) d\mathbf{x} = \oint_{\partial\Omega} p \mathbf{f} \cdot d\mathbf{S} \quad (11)$$

$$= \int_{\Omega} p \nabla \cdot \mathbf{f} d\mathbf{x} + \int_{\Omega} \mathbf{f} \cdot \nabla p d\mathbf{x} \quad (12)$$

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

$$\int_{\Omega} p \nabla \cdot \mathbf{f} d\mathbf{x} = - \int_{\Omega} \mathbf{f} \cdot \nabla p d\mathbf{x}. \quad (13)$$

or in summation form:

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

## 1.3 Probability Current (NOT FINISHED)

A general probability current is defined as

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

where  $W(\mathbf{x}' | \mathbf{x})$  is the transition probability kernel of the transition from a state  $\mathbf{x} \rightarrow \mathbf{x}'$  and  $W(\mathbf{x} | \mathbf{x}')$  is the transition probability kernel of its reverse  $\mathbf{x}' \rightarrow \mathbf{x}$ . The entries of  $W(\mathbf{x}' | \mathbf{x})$  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):

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

## 1.4 Interchanging Expectation and Derivative

### 1.4.1 Ansatz: Difference Quotient

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

$$\frac{\partial}{\partial t} \mathbb{E}[g(t, x)] = \lim_{h \rightarrow 0} \frac{1}{h} \left( \mathbb{E}[g(t+h, x)] - \mathbb{E}[g(t, x)] \right) \quad (17)$$

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

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

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

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

and thus we can use the Dominated Convergence Theorem to conclude

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

### 1.4.2 Ansatz: Leibnitz Rule

Suppose

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

We want to evaluate:

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

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,

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

$$\frac{dF}{dt} = \frac{d \langle g(\mathbf{x}(t)) \rangle}{dt} = \int_{\Omega} g(\mathbf{x}) \frac{\partial p(\mathbf{x}, t)}{\partial t} d\mathbf{x} \quad (25)$$

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:

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

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

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

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

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

## 1.5 Wiener Processes

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

1. Initial condition:

$$w(0) = 0 \quad (\text{almost surely}) \quad (27)$$

2. Independent increments: For any  $0 \leq t_1 < t_2 < \dots < t_n$ ,

$$w(t_{k+1}) - w(t_k) \text{ are independent random variables} \quad (28)$$

3. Gaussian increments:

$$w(t) - w(s) \sim \mathcal{N}(0, t - s) \quad \text{for } t > s \geq 0 \quad (29)$$

4. Continuous paths:

$$t \mapsto w(t) \text{ is almost surely continuous} \quad (30)$$

## 1.6 Ito SDE

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

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

where:

- $\mathbf{a} : \mathbb{R}^n \times [0, \infty) \rightarrow \mathbb{R}^n$  is the drift vector (deterministic component)
- $\mathbf{B} : \mathbb{R}^n \times [0, \infty) \rightarrow \mathbb{R}^{n \times m}$  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:

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



## 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

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

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

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

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

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

where  $dw_k dw_l = \delta_{kl} dt$  was used and higher-order terms involving  $dt dt$  and  $dt dw_k$  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:

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

## 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  $\mathbf{x} = (x_1, \dots, x_N)^T$  is given by

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

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 [3]. Note that some papers instead use the diffusion tensor  $\mathbf{D}(\mathbf{x}, t) = \mathbf{B}(\mathbf{x}, t) \mathbf{B}(\mathbf{x}, t)^T / 2$  [5].

## 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](#)):

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

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

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

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](#)):

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

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

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

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](#)):

$$\langle f \rangle = \int p f d\mathbf{x} \quad (43)$$

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

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

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

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  $p \mathbf{a} \cdot \nabla f$ :

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

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

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

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

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

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

where  $(:)$  denotes the double dot product

Substituting both expressions yields

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

Because the boundary is infinity but arbitrary

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

and because  $f$  is also arbitrary

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

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

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:

$$\begin{aligned} \frac{\partial p}{\partial t} &= -\nabla \cdot \mathbf{j}(\mathbf{x}, t) \\ \mathbf{j}(\mathbf{x}, t) &= p(\mathbf{x}, t)\mathbf{a}(\mathbf{x}, t) - \frac{1}{2} \nabla \cdot (\mathbf{B}(\mathbf{x}, t)\mathbf{B}(\mathbf{x}, t)^T p(\mathbf{x}, t)) \end{aligned} \quad (55)$$

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

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

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 Kolmogorov Backward Equation

Let  $F$  be a martingale  $F(\mathbf{x}, t) = \mathbb{E}[\phi(\mathbf{x}_T) | \mathbf{x}_t = \mathbf{x}]$ , where  $\phi(\mathbf{x}_T)$  is the final distribution at time  $T$ , which reads that  $F(\mathbf{x}, t)$  is the conditional probability that we arrive at  $\mathbf{x}_T$  at time  $T$ , given that the state at time  $t$  is  $\mathbf{x}_t = \mathbf{x}$ . Let  $F(\mathbf{x}, t)$  satisfy the boundary value problem

$$\frac{\partial F}{\partial t} + \nabla F \cdot \mathbf{a} + \frac{1}{2} \text{Tr}(\mathbf{B}\mathbf{B}^T \nabla^2 F) = 0, \quad F(\mathbf{x}, T) = F(\mathbf{x}_T, T) = \phi(\mathbf{x}_T)$$

Using Ito's Lemma, we obtain the total differential

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

Integrating both sides from  $t$  to  $T$ :

$$F(\mathbf{x}_T, T) - F(\mathbf{x}_t, t) = \int_t^T \left( \frac{\partial F}{\partial \tau} + \nabla F \cdot \mathbf{a} + \frac{1}{2} \text{Tr}(\mathbf{B}\mathbf{B}^T \nabla^2 F) \right) d\tau + \int_t^T (\nabla \phi \cdot \mathbf{B}) d\mathbf{w}$$

Because  $F(\mathbf{x}, \tau)$  solves the PDE, the term under the integral is 0. The conditional expectation of the Ito integral is also 0. Take the conditional expectation  $\mathbb{E}[(\cdot) | \mathbf{x}_t = \mathbf{x}]$  on both sides:

$$\mathbb{E}[F(\mathbf{x}_T, T) | \mathbf{x}_t = \mathbf{x}] = \mathbb{E}[F(\mathbf{x}_t, t) | \mathbf{x}_t = \mathbf{x}] = F(\mathbf{x}_t, t)$$

which means that  $F(\mathbf{x}, t)$  is the conditional expectation value  $F(\mathbf{x}, t) = \mathbb{E}[\phi(\mathbf{x}_T) | \mathbf{x}_t = \mathbf{x}]$  (the expectation of the function  $\phi(\mathbf{x}_T)$  at time  $T$ , given that is at  $\mathbf{x}_t$  at time  $t < T$ )

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

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

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

$$p_{\text{ESS}}(\mathbf{x}, t) = C e^{-\beta H(\mathbf{x})} = p_{\text{ESS}}(\mathbf{x}) \quad (57)$$

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

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

Using the product rule and the nice trick

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

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

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

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

$$\begin{aligned} \mathbf{a}(\mathbf{x}, t) &= \frac{1}{2} \mathbf{B} \mathbf{B}^T \nabla \ln(p_{\text{ESS}}(\mathbf{x}, t)) \\ &= \frac{1}{2} \mathbf{B} \mathbf{B}^T \nabla \ln(C e^{-\beta H(\mathbf{x})}) \\ &= -\frac{\beta}{2} \mathbf{B} \mathbf{B}^T \nabla (H(\mathbf{x})) \end{aligned} \tag{58}$$

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  $\rightarrow \mathbf{D} = \text{diag}(B_1^2, \dots, B_m^2)$

For this, take any row  $k$  from [Equation 58](#)

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

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:

$$B_k = \sqrt{-2 \langle a_k(\mathbf{x}, t) x_k \rangle} \tag{59}$$

## 2 TUR

### 2.1 Entropy production rate

#### 2.1.1 System Entropy production Rate

Gibbs entropy is defined as

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

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

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

Since integration and differentiation commute, the second integral vanishes:

$$\int \frac{\partial p(\mathbf{x}, t)}{\partial t} d\mathbf{x} = \frac{\partial}{\partial t} \int p(\mathbf{x}, t) d\mathbf{x} = \frac{\partial}{\partial t} (1) = 0 \quad (60)$$

so we are left with:

$$\boxed{\dot{S}_{\text{sys}}(t) = -k_B \int \frac{\partial p(\mathbf{x}, t)}{\partial t} \ln(p(\mathbf{x}, t)) d\mathbf{x}} \quad (61)$$

#### 2.1.2 Environment Entropy Production Rate (NOT FINISHED)

The environment's entropy production rate is given by

$$\dot{S}_{\text{env}} = \frac{1}{T} \int \mathbf{j}(\mathbf{x}, t) \cdot \mathbf{f}(\mathbf{x}, t) d\mathbf{x} \quad (62)$$

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

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

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

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

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

$$\begin{aligned} \dot{S}_{\text{tot}} &= -k_B \int \mathbf{j}(\mathbf{x}, t) \nabla \ln(p(\mathbf{x}, t)) + \frac{1}{T} \int \mathbf{j}(\mathbf{x}, t) \cdot \mathbf{f}(\mathbf{x}, t) d\mathbf{x} \\ &= \int \mathbf{j}(\mathbf{x}, t) \cdot \left( -k_B \frac{\nabla p(\mathbf{x}, t)}{p(\mathbf{x}, t)} + \frac{1}{T} \mathbf{f}(\mathbf{x}, t) \right) d\mathbf{x} \end{aligned} \quad (63)$$

### 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](#)):

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

Assume that the diffusion tensor is constant. In thermal equilibrium relates mobility and diffusion via  $\boldsymbol{\mu} = k_B T \mathbf{D}$  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

$$\mathbf{j}(\mathbf{x}, t) = \boldsymbol{\mu} (p(\mathbf{x}, t)\tilde{\mathbf{a}}(\mathbf{x}, t) - k_B T \nabla p(\mathbf{x}, t))$$

In this case, the thermodynamic force is the drift  $\mathbf{a}(\mathbf{x}, t)$ . Substituting the expression for the probability current into [Equation 63](#) yields:

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

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

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

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

$$\begin{aligned} \dot{S}_{\text{tot}} = \int & \left( p(\mathbf{x}, t) \left( \frac{\mathbf{j}(\mathbf{x}, t)}{p(\mathbf{x}, t)} + \mathbf{D} \frac{\nabla p(\mathbf{x}, t)}{p(\mathbf{x}, t)} \right) - \mathbf{D} \nabla p(\mathbf{x}, t) \right) \\ & \cdot \left( -k_B \frac{\nabla p(\mathbf{x}, t)}{p(\mathbf{x}, t)} + \frac{1}{T} \left( \frac{\mathbf{j}(\mathbf{x}, t)}{p(\mathbf{x}, t)} + \mathbf{D} \frac{\nabla p(\mathbf{x}, t)}{p(\mathbf{x}, t)} \right) \right) d\mathbf{x} \\ = \int & \frac{\mathbf{j}(\mathbf{x}, t)}{p(\mathbf{x}, t)} \cdot \left( -k_B \nabla p(\mathbf{x}, t) + \frac{1}{T} (\mathbf{j}(\mathbf{x}, t) + \mathbf{D} \nabla p(\mathbf{x}, t)) \right) d\mathbf{x} \end{aligned} \quad (64)$$

$$(65)$$

## 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):

$$I(j) \leq \sum_{y < z} \frac{(j(y, z) - j^\pi(y, z))^2}{4j^\pi(y, z)} \sigma^\pi(y, z),$$

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  $\Sigma^\pi$ , 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  $I(j_d)$ :

$$\text{Var}(j_d) = \frac{1}{I''(j_d^\pi)}.$$



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:

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

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

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

or equivalently, the **relative uncertainty**  $\epsilon_d^2 = \text{Var}(j_d)/(j_d^\pi)^2$  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  $\Sigma$ .
- 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  $\Sigma^\pi$  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 [3])

### 2.3.1 Assumptions

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

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

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

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

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

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  $\theta$  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  $\theta$  perturbation, derive the fluctuation-response inequality as:

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

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

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

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  $\theta$ :

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

where  $D_{\text{PE}}$  is the Pearson divergence. Generalizable via Chapman-Robbins inequality

### 3 Circuit Theory Stuff

#### 3.1 Node Flux

Define the node flux  $\phi$ , which is connected to the voltage  $U$  via

$$\dot{\phi} = U \quad (66)$$

Motivation from 2nd Maxwell equation:

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

Equations for ohmic resistor, capacitor, coil:

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

$$\dot{\phi}_R = RI_R = U_R$$

- Coil (stores energy in magnetic field as current  $I_L$ ):

$$\begin{aligned} \dot{\phi}_L &= L \frac{dI_L}{dt} = U_L \quad \rightarrow \quad \phi_L = LI_L \\ H_L &= \frac{1}{2} LI_L^2 = \frac{\phi_L^2}{2L} \end{aligned}$$

- Capacitor (stores energy in electric field as charge  $Q_C$ ):

$$\begin{aligned} I_C &= C \ddot{\phi}_C = C \frac{dU_C}{dt} \\ H_C &= \frac{1}{2} CU_C^2 = \frac{Q_C^2}{2C} \end{aligned}$$

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

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

#### 3.2 Thermal Bath Coupling

$$H_{\text{bath}} = \sum_k \left( \frac{p_k^2}{2m_k} + \frac{1}{2} m_k \omega_k^2 q_k^2 \right) \quad (67)$$

$$= \sum_k \hbar \omega_k \left( a_k^\dagger a_k + \frac{1}{2} \right) \quad (68)$$

$$H_{\text{coupling}} = -A \sum_k c_k q_k \tag{69}$$

$$= A \sum_k g_k \left( b_k^\dagger + b_k \right) \tag{70}$$

## 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 explicitly 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

$$x_i(t_{n+1}) = x_i(t_n) + \int_{t_n}^{t_n + \Delta t} a_i(\mathbf{x}(t)) dt + \sum_{j=1}^M \int_{t_n}^{t_n + \Delta t} B_{ij}(\mathbf{x}(t)) dw_j(t) \quad (71)$$

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

$$\|\mathbf{a}(\mathbf{x})\|^2 \leq K_{\mathbf{a}}(1 + \|\mathbf{x}\|^2) \quad (72)$$

$$\|\mathbf{B}(\mathbf{x})\|^2 \leq K_{\mathbf{B}}(1 + \|\mathbf{x}\|^2) \quad (73)$$

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  $\gamma$  if

$$\boxed{\mathbb{E} [\|\mathbf{x}(t_n) - \mathbf{x}_n\|] = \mathcal{O}(\Delta t^\gamma)} \quad (74)$$

where  $x(t_n)$  is the exact solution at time  $t_n$  and  $x_n$  is the approximate solution at  $t_n = \tau$  [4].

#### 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  $\beta$  if for all smooth test functions  $\phi$  it satisfies

$$\boxed{|\mathbb{E}[\phi(\mathbf{x}(t_n))] - \mathbb{E}[\phi(\mathbf{x}_n)]| = \mathcal{O}(\Delta t^\beta)} \quad (75)$$

where  $x(t_n)$  is the exact solution at time  $t_n$  and  $x_n$  is the approximate solution at  $t_n = \tau$  [4].

## 4.2 Euler-Maruyama (Euler-Forward)

Solve the integrals from Equation 71 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:

$$\begin{aligned} x_i(t_n + \Delta t) &\approx x_i(t_n) + \int_{t_n}^{t_n + \Delta t} a_i(\mathbf{x}(t_n)) d\tau + \sum_{j=1}^M \int_{t_n}^{t_n + \Delta t} B_{ij}(\mathbf{x}(t_n)) dw_j(\tau) \\ &= x_i(t_n) + a_i(\mathbf{x}(t_n)) \Delta t + \sum_{j=1}^M B_{ij}(\mathbf{x}(t_n)) (w_j(t_n + \Delta t) - w_j(t_n)) \end{aligned} \quad (76)$$

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

$$x_i^{n+1} = x_i^n + a_i(\mathbf{x}_n) \Delta t + \sum_{j=1}^M B_{ij}(\mathbf{x}_n) (w_j^{n+1} - w_j^n) \quad (77)$$

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \mathbf{a}(\mathbf{x}_n) \Delta t + \mathbf{B}(\mathbf{x}_n) (\mathbf{w}_{n+1} - \mathbf{w}_n) \quad (78)$$

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 $\leq 0 \rightarrow$ evaluate again!!)

The error at  $t_{n+1}$  is

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

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

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

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 constant

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

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 constant

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



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

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

$$\mathbb{E}[\mathbf{e}_n \cdot \mathbf{u}_n] = \nabla \mathbf{a} \Big|_{\mathbf{x}_n} \mathbb{E}[\|\mathbf{e}_n\|^2] \Delta t + (\text{higher-order terms})$$

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

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

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

$$\mathbb{E}[\|\mathbf{u}_n\|^2] = (\nabla \mathbf{a} \Big|_{\mathbf{x}_n})^2 \mathbb{E}[\|\mathbf{e}_n\|^2] \Delta t^2 + (\text{higher-order terms})$$

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

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

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

$$\mathbb{E}[\|\mathbf{v}_n\|^2] = (\nabla \mathbf{B} \Big|_{\mathbf{x}_n})^2 \mathbb{E}[\|\mathbf{e}_n\|^2] \Delta t + (\text{higher-order terms})$$

Putting everything together:

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

#### 4.2.2 Weak Convergence Order

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

$$|\mathbb{E}[\phi(\mathbf{x}(t_n))] - \mathbb{E}[\phi(\mathbf{x}_n)]|. \quad (79)$$

Writing  $\langle \cdot \rangle$ , substituting the exact solution from ?? over a time interval  $[t_n, t_n + \Delta t]$  and substituting the approximate solution from Equation 78, we get

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

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

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

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

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

And thus

$$|\mathbb{E}[\phi(\mathbf{x}(t_n))] - \mathbb{E}[\phi(\mathbf{x}_n)]| \leq C' \Delta t \quad (80)$$

### 4.2.3 Implementation

Implementation of the forward Euler method (see [Equation 78](#)): 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:

$$\underbrace{\left[ M \left\{ \overbrace{\left( \Delta \mathbf{w}_1^{(1)} \cdots \Delta \mathbf{w}_1^{(N_s)} \right)}^{N_s}, \cdots \left( \Delta \mathbf{w}_{N_t}^{(1)} \cdots \Delta \mathbf{w}_{N_t}^{(N_s)} \right) \right\} \right]}_{N_t \text{ matrices}} \quad (81)$$

Vectorize updating the solution:

$$\mathbf{X}_n = \underbrace{\left[ \mathbf{x}_n^{(1)} \cdots \mathbf{x}_n^{(N_s)} \right]}_{N_s} \Bigg\} N \quad (82)$$

$$\mathbf{A}(\mathbf{X}_n) = \underbrace{\left[ \mathbf{a}(\mathbf{x}_n^{(1)}) \cdots \mathbf{a}(\mathbf{x}_n^{(N_s)}) \right]}_{N_s} \Bigg\} N \quad (83)$$

Less expensive to loop over state dimensions  $N$  than MC steps

$$\mathbf{B}(\mathbf{X}_n) = \underbrace{\left[ N_s \left\{ \overbrace{\left( \begin{pmatrix} \mathbf{B}_{11}(\mathbf{x}_n^{(1)}) & \cdots & \mathbf{B}_{1M}(\mathbf{x}_n^{(1)}) \\ \vdots & & \vdots \\ \mathbf{B}_{11}(\mathbf{x}_n^{(N_s)}) & \cdots & \mathbf{B}_{1M}(\mathbf{x}_n^{(N_s)}) \end{pmatrix})}^M, \cdots \left( \begin{pmatrix} \mathbf{B}_{N1}(\mathbf{x}_n^{(1)}) & \cdots & \mathbf{B}_{NM}(\mathbf{x}_n^{(1)}) \\ \vdots & & \vdots \\ \mathbf{B}_{N1}(\mathbf{x}_n^{(N_s)}) & \cdots & \mathbf{B}_{NM}(\mathbf{x}_n^{(N_s)}) \end{pmatrix}) \right\} \right]}_{N \text{ matrices}} \quad (84)$$

### 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:

$$\begin{aligned} B_{ij}(\mathbf{x}(t)) &\approx B_{ij}(\mathbf{x}_n) + \left. \frac{\partial B_{ij}(\mathbf{x})}{\partial t} \right|_{\mathbf{x}_n} (t - t_n) \\ &\quad + \sum_{k=1}^N \left. \frac{\partial B_{ij}(\mathbf{x})}{\partial x_k} \right|_{\mathbf{x}_n} (x_k(t) - x_k(t_n)) + (\text{higher order terms}) \end{aligned} \quad (85)$$

Substituting this expression into the integral in [Equation 71](#) yields:

$$\begin{aligned} \int_{t_n}^{t_n+\Delta t} B_{ij}(\mathbf{x}) dw_j(t) &\approx B_{ij}(\mathbf{x}_n) \int_{t_n}^{t_n+\Delta t} dw_j(t) \\ &\quad + \sum_{k=1}^N \left. \frac{\partial B_{ij}(\mathbf{x})}{\partial x_k} \right|_{\mathbf{x}_n} \int_{t_n}^{t_n+\Delta t} (x_k(t) - x_k(t_n)) dw_j(t) \\ &\quad + \left. \frac{\partial B_{ij}(\mathbf{x})}{\partial t} \right|_{\mathbf{x}_n} \int_{t_n}^{t_n+\Delta t} (t - t_n) dw_j(t) \end{aligned} \quad (86)$$

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

$$x_k(t) \approx x_k(t_n) + a_k(\mathbf{x}(t_n))(t - t_n) + \sum_{l=1}^M \int_{t_n}^t B_{kl}(\mathbf{x}(t)) dw_l(t) \quad (87)$$

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

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

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

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

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

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

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

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

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

$$\begin{aligned} x_i^{n+1} &= x_i^n + a_i(\mathbf{x}_n) \Delta t + \sum_{j=1}^M B_{ij}(\mathbf{x}_n) (w_j^{n+1} - w_j^n) \\ &+ \frac{1}{2} \sum_{k=1}^N \frac{\partial B_{ij}^n}{\partial x_k} B_{kj}^n ((w_j^{n+1} - w_j^n)^2 - \Delta t) \end{aligned} \quad (88)$$

## 4.4 Finite Volume Method for solving the Fokker-Planck Equation

### 4.4.1 1D Case

#### Spatial Discretization

The Fokker-Planck equation (FPE) in 1D is:

$$\frac{\partial p(x, t)}{\partial t} = - \frac{\partial j(x, t)}{\partial x},$$

where the probability current  $j(x, t)$  is:

$$j(x, t) = a(x)p(x, t) - \frac{\partial}{\partial x} [D(x)p(x, t)].$$

Divide the domain into  $N$  control volumes centered at  $x_i, i = 1, \dots, N$  with uniform spacing  $\Delta x$ . Cell faces are at:

$$x_{i\pm 1/2} = x_i \pm \Delta x/2.$$

Integrate the FPE over the  $i$ -th cell  $[x_{i-1/2}, x_{i+1/2}]$ :

$$\begin{aligned} \int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial p(x, t)}{\partial t} dx &= - \int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial j(x, t)}{\partial x} dx \stackrel{\text{Divergence Theorem}}{=} - (j_{i+1/2} - j_{i-1/2}) \\ &\approx \Delta x \frac{\partial p_i}{\partial t} \end{aligned}$$

The current  $j_{i+1/2}$  is approximated as (central differences):

$$\begin{aligned} j_{i+1/2} &= a(x_{i+1/2}) \left( \frac{p_i + p_{i+1}}{2} \right) - \frac{D(x_{i+1})p_{i+1} - D(x_i)p_i}{\Delta x}, \\ j_{i-1/2} &= a(x_{i-1/2}) \left( \frac{p_{i-1} + p_i}{2} \right) - \frac{D(x_i)p_i - D(x_{i-1})p_{i-1}}{\Delta x}. \end{aligned}$$

Or via the upwind scheme:

$$p_i + p_{i+1} \frac{D(x_{i+1})p_{i+1} - D(x_i)p_i}{2 - \frac{D(x_{i+1})p_{i+1} - D(x_i)p_i}{\Delta x}}, j_{i-1/2} = a(x_{i-1/2}) \left( \frac{p_{i-1} + p_i}{2} \right) - \frac{D(x_i)p_i - D(x_{i-1})p_{i-1}}{\Delta x}.$$

### Temporal Discretization

Using forward Euler:

$$p_i^{n+1} = p_i^n - \frac{\Delta t}{\Delta x} (j_{i+1/2}^n - j_{i-1/2}^n).$$

The time step must satisfy (can be derived via Von-Neumann-stability analysis (Fourier space)):

$$\Delta t \leq \min \left( \frac{\Delta x}{\max |a(x)|}, \frac{\Delta x^2}{2 \max D(x)} \right).$$

### Boundary Conditions

No-Flux:

$$j_{1/2} = j_{N+1/2} = 0 \quad \Rightarrow \quad p_0^n = p_1^n, \quad p_{N+1}^n = p_N^n.$$

Periodic:

$$j_{1/2} = j_{N+1/2}, \quad p_0^n = p_N^n, \quad p_{N+1}^n = p_1^n.$$

The full discretized scheme is:

$$p_i^{n+1} = p_i^n - \frac{\Delta t}{\Delta x} (j_{i+1/2}^n - j_{i-1/2}^n),$$

where  $j_{i+1/2}^n = a(x_{i+1/2}) \left( \frac{p_i^n + p_{i+1}^n}{2} \right) - \frac{D(x_{i+1})p_{i+1}^n - D(x_i)p_i^n}{\Delta x}$

and  $j_{i-1/2}^n = a(x_{i-1/2}) \left( \frac{p_{i-1}^n + p_i^n}{2} \right) - \frac{D(x_i)p_i^n - D(x_{i-1})p_{i-1}^n}{\Delta x}$

## 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 ( $\mathbf{B}(\mathbf{x}, t) = B$ )

$$\dot{x} = B\xi(t). \quad (89)$$

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

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

$$\begin{aligned} \dot{x}(t) &= B\xi(t) \\ x(t) &= B \int_0^t \xi(t') dt' \\ \langle x(t) \rangle &= B \int_0^t \langle \xi(t') \rangle dt' = B \int_0^t 0 dt' = 0 \end{aligned} \quad (90)$$

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

$$\begin{aligned} x^2(t) &= \left( B \int_0^t \xi(t') dt' \right)^2 = B^2 \int_0^t \int_0^t \xi(t') \xi(t'') dt' dt'' \\ \langle x^2(t) \rangle &= \left\langle B^2 \int_0^t \int_0^t \xi(t') \xi(t'') dt' dt'' \right\rangle = B^2 \int_0^t \int_0^t \langle \xi(t') \xi(t'') \rangle dt' dt'' \\ &= B^2 \int_0^t \int_0^t \delta(t'' - t') dt' dt'' = B^2 \int_0^t dt'' = B^2 t \end{aligned} \quad (91)$$

The variance is then

$$\langle \langle x(t) \rangle \rangle = \langle x^2(t) \rangle - \langle x(t) \rangle^2 = B^2 t - 0 = B^2 t \quad (92)$$

#### 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

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

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

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

### 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:

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

3. Inverse Fourier transform back into state space

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

4. perform quadratic completion

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

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

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

5. Solve integral with error function

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

6. Final solution:

$$p(x, t) = \frac{1}{\sqrt{2\pi B^2 t}} e^{-\frac{(x-x_0)^2}{2B^2 t}} \quad (93)$$

This is the PDF of a Gaussian distribution with

$$\langle x(t) \rangle = x_0 \quad (94)$$

$$\langle \langle x(t) \rangle \rangle = \langle x^2(t) \rangle - \langle x(t) \rangle^2 = B^2 t \quad (95)$$

### 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:

$$\dot{\hat{x}}(\hat{t}) = \frac{d(x_0 \hat{x})}{d\hat{t}} \frac{d\hat{t}}{dt} = \frac{x_0}{t_0} \frac{d\hat{x}}{d\hat{t}} = B \frac{\xi(\hat{t})}{\sqrt{t_0}} \quad (96)$$

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

$$\dot{\hat{x}}(\hat{t}) = \xi(\hat{t}) \quad (97)$$

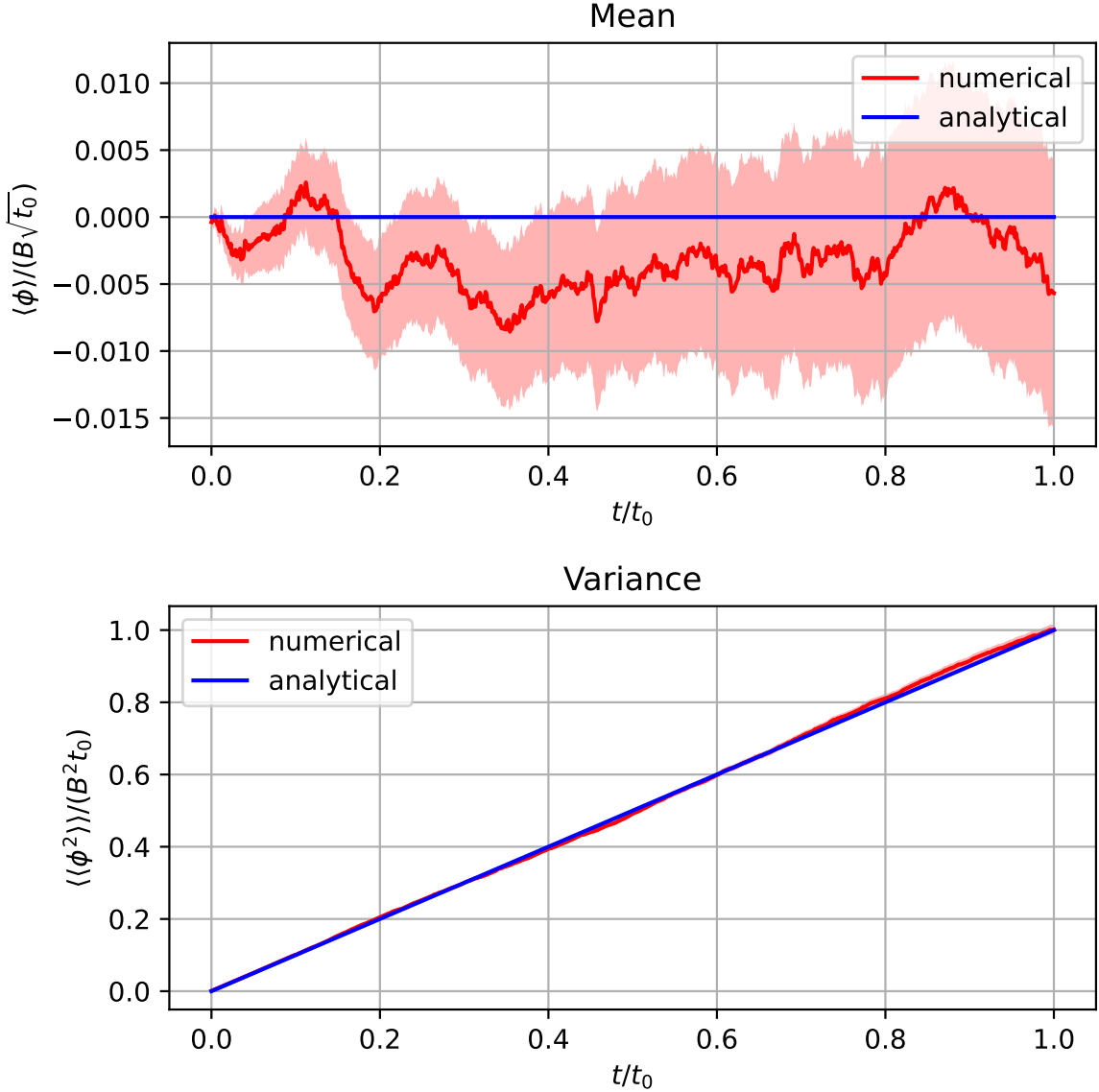


Figure 1:  $\hat{T} = 1$ ,  $N_t = 10^4$  time steps.  $N_s = 10^4$  MC-steps (ensemble-realizations). The shaded region corresponds to the  $1\sigma$ -interval



## 5.2 LR Circuit with Current Source

Consider an electrical circuit consisting of

- Ohmic Resistor:

$$\dot{\phi}_R = RI_R = U_R \quad (98)$$

- Coil:

$$\dot{\phi}_L = L \frac{dI_L}{dt} = U_L \quad \rightarrow \quad \phi_L = LI_L \quad (99)$$

- Current Source  $I_0$

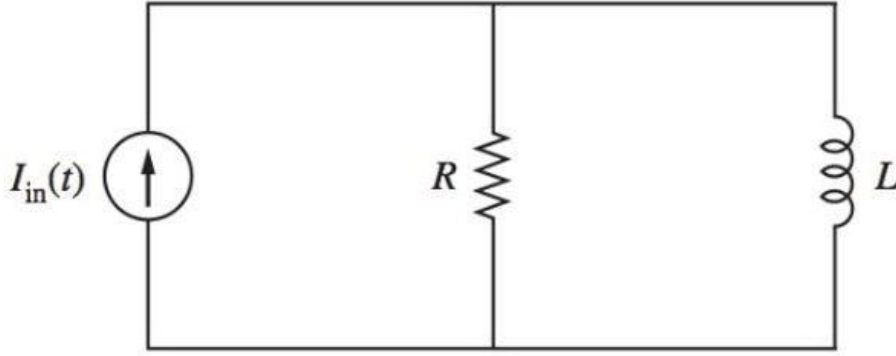


Figure 2: LR Circuit

Kirchhoff's rules yield:

$$U_R = U_L \quad (100)$$

$$I_R + I_L = I_0 \quad (101)$$

Substituting node flux for current and voltage results in

$$I_R + I_L = \frac{\dot{\phi}_R}{R} + \frac{\phi_L}{L} = I_0 \quad (102)$$

since Maxwell's equations are gauge-invariant, we can say that from  $\dot{\phi}_R = \dot{\phi}_L \rightarrow \phi_R = \phi_L = \phi$ . This results in the ODE

$$\frac{\dot{\phi}}{R} + \frac{\phi}{L} = I_0 \quad (103)$$

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

$$\dot{\phi} = -\frac{R}{L}\phi + B\xi(t). \quad (104)$$

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 59) to obtain the consistent diffusion term  $B$ : With

$$\langle A(x, t) \rangle = - \left\langle \frac{R}{L} \phi^2 \right\rangle = -2R \left\langle \frac{\phi^2}{2L} \right\rangle = -R H_L = -R \left\langle \phi \frac{d}{d\phi} \frac{\phi^2}{2L} \right\rangle = -R \left\langle \phi \frac{d}{d\phi} H_L \right\rangle \quad (105)$$

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

$$\langle A(x, t) \rangle = - \frac{R}{\beta} \quad (106)$$

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

$$B = \sqrt{-2 \langle A(x, t) \rangle} = \sqrt{2Rk_B T} \quad (107)$$

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

$$\phi(t) = \phi(0)e^{-\frac{R}{L}t} + B \int_0^t e^{-\frac{R}{L}(t-\tau)} \xi(\tau) d\tau \quad (108)$$

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,

$$\begin{aligned} \langle \phi(t) \rangle &= \left\langle \phi(0)e^{-\frac{R}{L}t} \right\rangle + B \int_0^t e^{-\frac{R}{L}(t-\tau)} \langle \xi(\tau) \rangle d\tau = \\ &= \phi(0)e^{-\frac{R}{L}t} \end{aligned} \quad (109)$$

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

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

Taking the expectation on both sides

$$\begin{aligned}
\langle \phi^2(t) \rangle &= \left\langle \phi^2(0) e^{-\frac{2R}{L}t} \right\rangle + B^2 \int_0^t \int_0^t e^{-\frac{R}{L}(t-\tau)} e^{-\frac{R}{L}(t-\tau')} \langle \xi(\tau) \xi(\tau') \rangle d\tau d\tau' \\
&= \phi^2(0) e^{-\frac{2R}{L}t} + B^2 \int_0^t \int_0^t e^{-\frac{R}{L}(t-\tau)} e^{-\frac{R}{L}(t-\tau')} \delta(\tau - \tau') d\tau d\tau' \\
&= \phi^2(0) e^{-\frac{2R}{L}t} + B^2 \int_0^t e^{-\frac{2R}{L}(t-\tau)} d\tau \\
&= \phi^2(0) e^{-\frac{2R}{L}t} + \frac{B^2 L}{2R} \left( 1 - e^{-\frac{2R}{L}t} \right)
\end{aligned} \tag{110}$$

The variance is then

$$\begin{aligned}
\langle \langle \phi(t) \rangle \rangle &= \langle \phi^2(t) \rangle - \langle \phi(t) \rangle^2 = \phi^2(0) e^{-\frac{2R}{L}t} + \frac{B^2 L}{2R} \left( 1 - e^{-\frac{2R}{L}t} \right) - \phi^2(0) e^{-\frac{2R}{L}t} \\
&= \frac{B^2 L}{2R} \left( 1 - e^{-\frac{2R}{L}t} \right) = k_B T L \left( 1 - e^{-\frac{2R}{L}t} \right)
\end{aligned} \tag{111}$$

In summary:

$$\boxed{\langle \phi(t) \rangle = \phi(0) e^{-\frac{R}{L}t}} \tag{112}$$

$$\boxed{\langle \langle \phi^2(t) \rangle \rangle = k_B T L \left( 1 - e^{-\frac{2R}{L}t} \right)} \tag{113}$$

### 5.2.3 Computing Mean and Variance via the Fokker-Planck Equation

The Fokker-Planck equation for this system reads

$$\frac{\partial p(\phi, t)}{\partial t} = \frac{R}{L} \frac{\partial}{\partial \phi} (\phi p) + \frac{1}{2} B^2 \frac{\partial^2 p}{\partial \phi^2} \tag{114}$$

$$p(\phi, 0) = \delta(\phi - \phi(0)) \tag{115}$$

Linear parabolic PDE: Solve using Fourier Transform

1. Transform in Fourier space:

$$\hat{p}(\omega, t) = \int_{-\infty}^{\infty} p(\phi, t) e^{-i\omega\phi} d\phi \tag{116}$$

$$\hat{p}(\omega, 0) = e^{-i\omega\phi_0} \tag{117}$$

2. In Fourier space, the PDE reads:

$$\frac{\partial \tilde{p}}{\partial t} = \frac{R}{L} \left( -i \frac{\partial}{\partial \omega} (\omega \tilde{p}) + \tilde{p} \right) - \frac{1}{2} B^2 \omega^2 \tilde{p} \tag{118}$$

3. Ansatz:

$$\tilde{p}(\omega, t) = e^{f(\omega, t)} \tag{119}$$

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

$$f(\omega, t) = -i\omega\phi(0)e^{-\frac{R}{L}t} - \frac{B^2L}{4R}\omega^2 \left(1 - e^{-\frac{2R}{L}t}\right) \quad (120)$$

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

$$\mu(t) = \phi(0)e^{-\frac{R}{L}t} \quad (121)$$

$$\sigma^2(t) = \frac{B^2L}{2R} \left(1 - e^{-\frac{2R}{L}t}\right) \quad (122)$$

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:

$$\dot{\phi}(\hat{t}) = \frac{d(\phi_0\varphi(\hat{t}))}{d\hat{t}} \frac{d\hat{t}}{dt} = \frac{\phi_0}{t_0} \frac{d\varphi(\hat{t})}{d\hat{t}} = -\frac{R}{L}\varphi(\hat{t})\phi_0 + \sqrt{2Rk_B T} \frac{\xi(\hat{t})}{\sqrt{t_0}} \quad (123)$$

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

$$\dot{\varphi}(\hat{t}) = -t_0 \frac{R}{L} \varphi(\hat{t}) + \frac{\sqrt{t_0}}{\phi_0} \sqrt{2Rk_B T} \xi(\hat{t}) \quad (124)$$

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

$$\dot{\varphi}(\hat{t}) = -\varphi(\hat{t}) + \xi(\hat{t}) \quad (125)$$

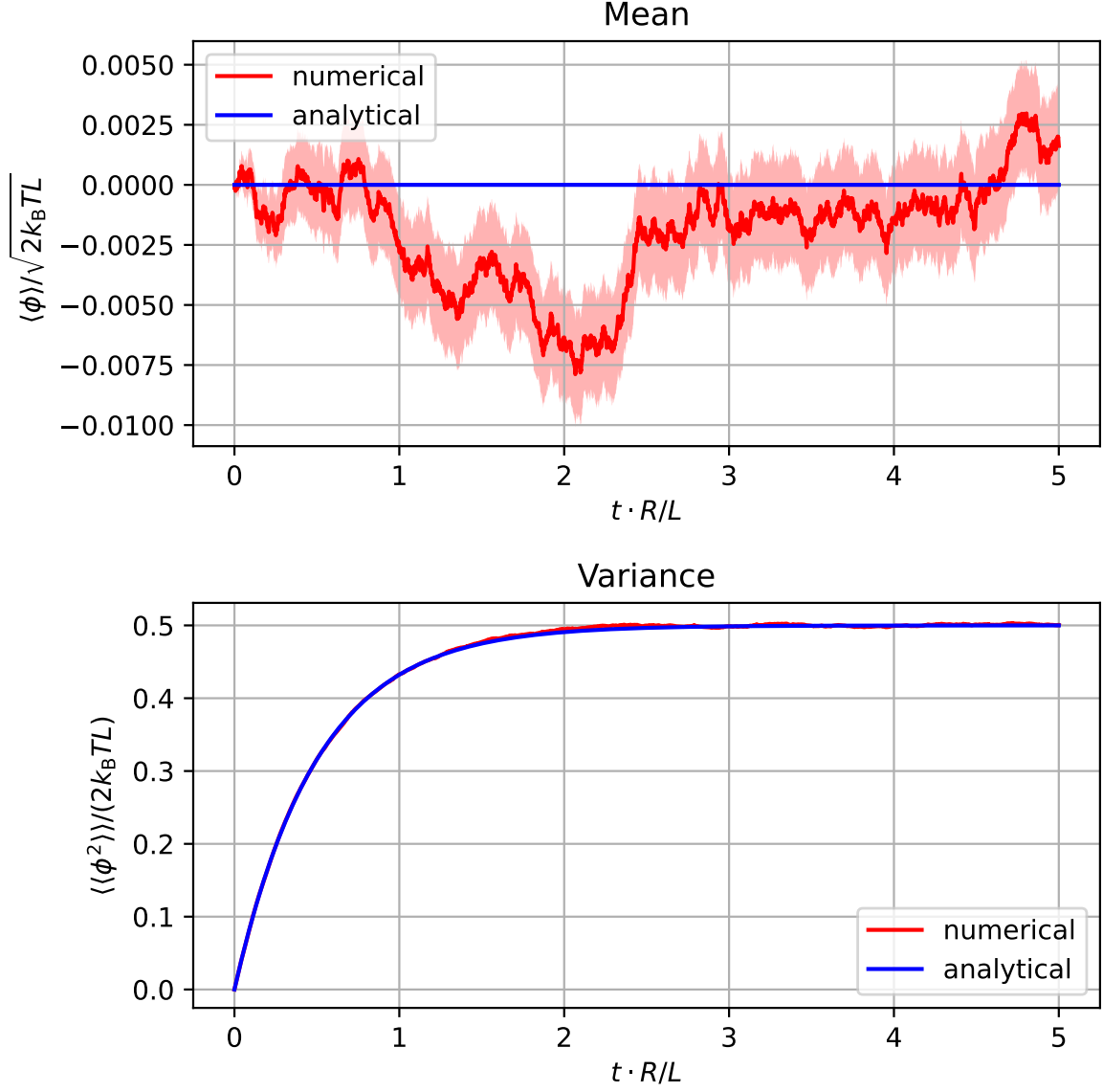


Figure 3:  $\hat{T} = 5$ ,  $N_t = 10^5$  time steps.  $N_s = 5 \cdot 10^3$  MC-steps (ensemble-realizations). The shaded region corresponds to the  $1\sigma$ -interval

### 5.3 Resistor with Current Source

Consider an electrical circuit consisting of

- Ohmic Resistor:

$$\dot{\phi}_R = RI_R = U_R \quad (126)$$

- Current Source  $I_0$

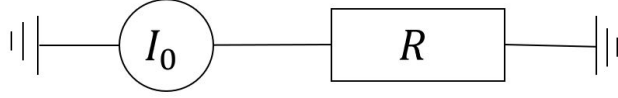


Figure 4: Resistor circuit

By using Kirchhoff's rules, we obtain the ODE

$$I_R = \frac{U_R}{R} = \frac{\dot{\phi}_R}{R} = I_0. \quad (127)$$

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](#))

$$\dot{\phi}_R = RI_0 + B\xi(t) \quad (128)$$

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  $B = \sqrt{2Rk_B T}$  (see [Equation 107](#)). Per convention, instead we use the notation  $B = \alpha/R$  with  $\alpha = \sqrt{2k_B T/R}$ , which yields the SDE

$$\dot{\phi}_R = RI_0 + \frac{\alpha}{R}\xi(t) \quad (129)$$

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

Integrating both sides with respect to time yields

$$\phi(t) = \int_0^t (RI_0 + \frac{\alpha}{R}\xi(t')) dt' \quad (130)$$

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

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

This yields the mean and variance

$$\boxed{\langle \phi(t) \rangle = RI_0 t} \tag{131}$$

$$\boxed{\langle \langle \phi^2(t) \rangle \rangle = 2Rk_B T t} \tag{132}$$

The node flux diverges as  $t \rightarrow \infty$ . 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  $\sigma$  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

$$\frac{\langle \langle \phi^2(t) \rangle \rangle}{\langle \phi(t) \rangle^2} \cdot \sigma t = \frac{2Rk_B T t}{R^2 I_0^2 t^2} \cdot \frac{RI_0^2}{T} t = 2k_B \geq 2k_B \tag{133}$$

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:

$$\dot{\phi}(\hat{t}) = \frac{d(\phi_0 \varphi(\hat{t}))}{d\hat{t}} \frac{d\hat{t}}{dt} = \frac{\phi_0}{t_0} \frac{d\varphi(\hat{t})}{d\hat{t}} = RI_0 + \sqrt{2Rk_B T} \frac{\xi(\hat{t})}{\sqrt{t_0}} \tag{134}$$

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

$$\dot{\varphi}(\hat{t}) = \frac{t_0}{\phi_0} RI_0 + \frac{\sqrt{t_0}}{\phi_0} \sqrt{2Rk_B T} \xi(\hat{t}) \tag{135}$$

Take the reference time and reference node flux  $t_0 = 2k_B T / (RI_0^2)$  and  $\phi_0 = 2k_B T / I_0$ , the SDE becomes

$$\dot{\varphi}(\hat{t}) = 1 + \xi(\hat{t}) \tag{136}$$

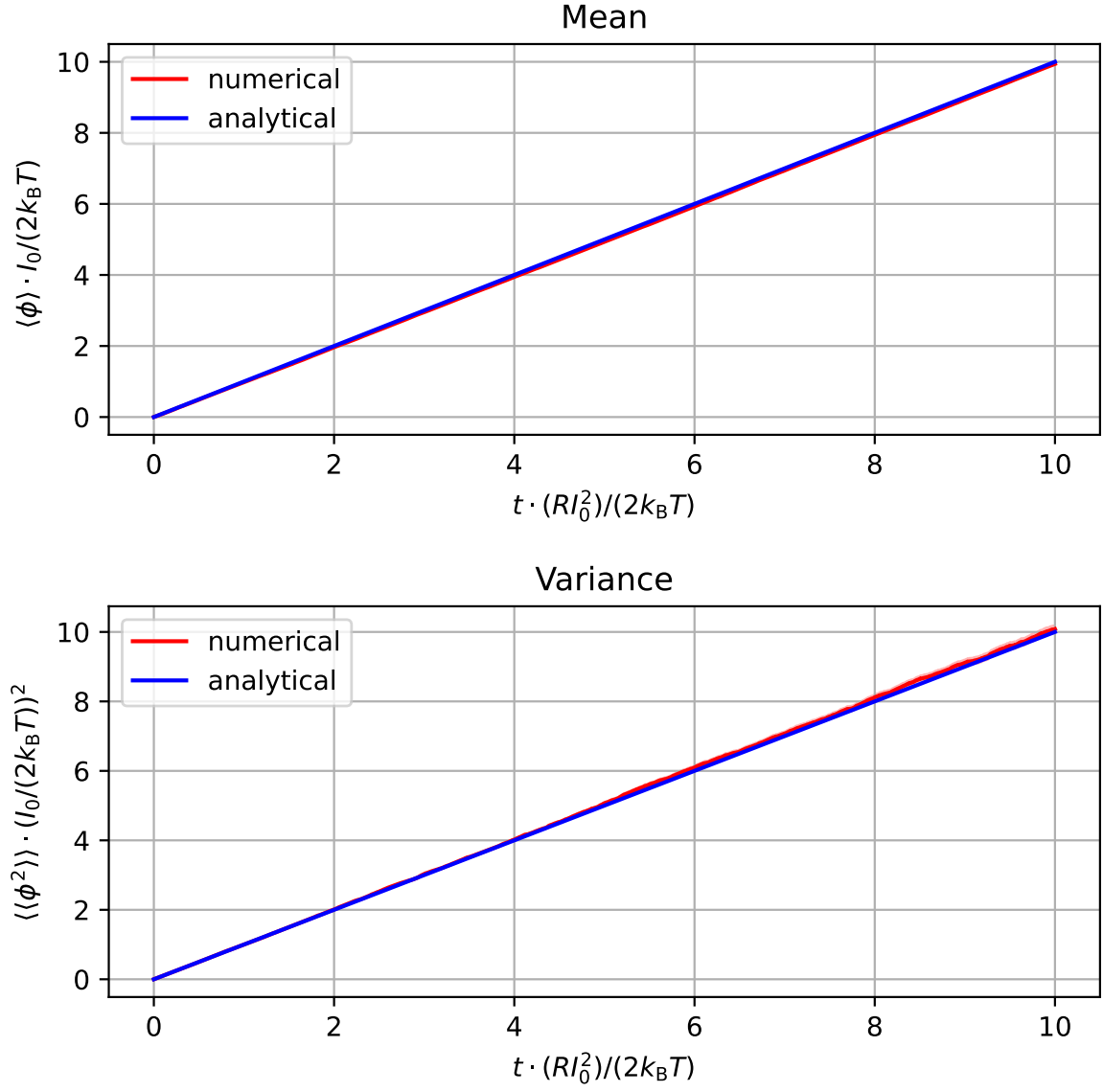


Figure 5:  $\hat{T} = 1$ ,  $N_t = 10^4$  time steps.  $N_s = 10^4$  MC-steps (ensemble-realizations). The shaded region corresponds to the  $1\sigma$ -interval



## 6 Overdamped RSJ Model

Consider a circuit made up of

- Ohmic Resistor

$$\dot{\phi}_R = RI_R = U_R$$

- Josephson Junction

$$I = I_c \sin\left(\frac{2e}{\hbar}\phi\right)$$

$$\dot{\phi} = V$$

- Current source  $I_0$

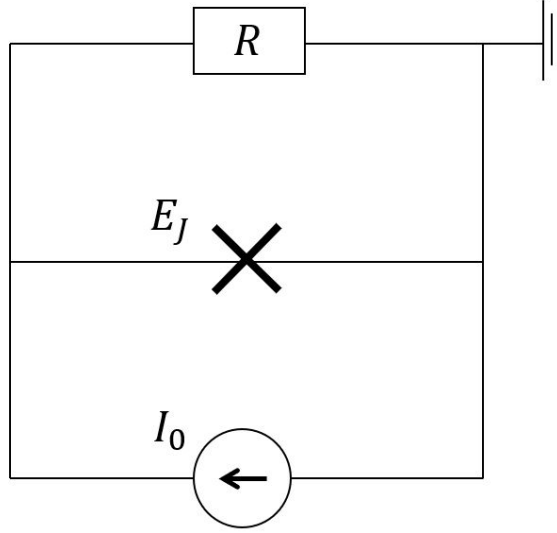


Figure 6: Circuit consisting of a Josephson junction and an ohmic resistor

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

$$I_0 + \sqrt{\frac{2k_B T}{R}} \xi(t) = \frac{\dot{\phi}}{R} + I_c \sin\left(\frac{2e}{\hbar}\phi\right)$$

Rearranging:

$$\dot{\phi} = RI_0 - RI_c \sin\left(\frac{2e}{\hbar}\phi\right) + \sqrt{2Rk_B T} \xi(t)$$

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

$$\dot{\phi}(\tau) = \frac{d(\phi_0 \varphi(\tau))}{d\tau} \frac{d\tau}{dt} = \frac{\phi_0}{t_0} \frac{d\varphi(\tau)}{d\tau} = RI_0 - RI_c \sin\left(\frac{2e}{\hbar} \phi_0 \varphi(\tau)\right) + \sqrt{2Rk_B T} \frac{\xi(\tau)}{\sqrt{t_0}}$$

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

$$\dot{\varphi}(\tau) = \frac{t_0}{\phi_0} R I_0 - \frac{t_0}{\phi_0} R I_c \sin\left(\frac{2e}{\hbar} \phi_0 \varphi(\tau)\right) + \frac{\sqrt{t_0}}{\phi_0} \sqrt{2 R k_B T} \xi(\tau)$$

Choosing  $\phi_0 = \hbar/(2e)$  and  $t_0 = \hbar/(2e R I_c) =: 1/\omega_G$  with  $G = 1/R$  and abbreviating  $I_0/I_c =: i_0$  leads to the dimensionless SDE

$$\dot{\varphi}(\tau) = i_0 - \sin(\varphi(\tau)) + \sqrt{\frac{4e k_B T}{\hbar I_c}} \xi(\tau) \quad (137)$$

The diffusion term can be expressed as

$$\sqrt{\frac{4e k_B T}{\hbar I_c}} = \sqrt{\frac{2 k_B T}{E_J}} \quad (138)$$

where  $E_J = \hbar I_c/(2e)$  is the Josephson energy. The term  $i_0 - \sin(\varphi)$  can be written as the gradient of the tilted washboard potential  $i_0 - \sin(\varphi) = -dU/d\varphi$  with  $U(\varphi) = -i_0\varphi - \cos(\varphi)$ .

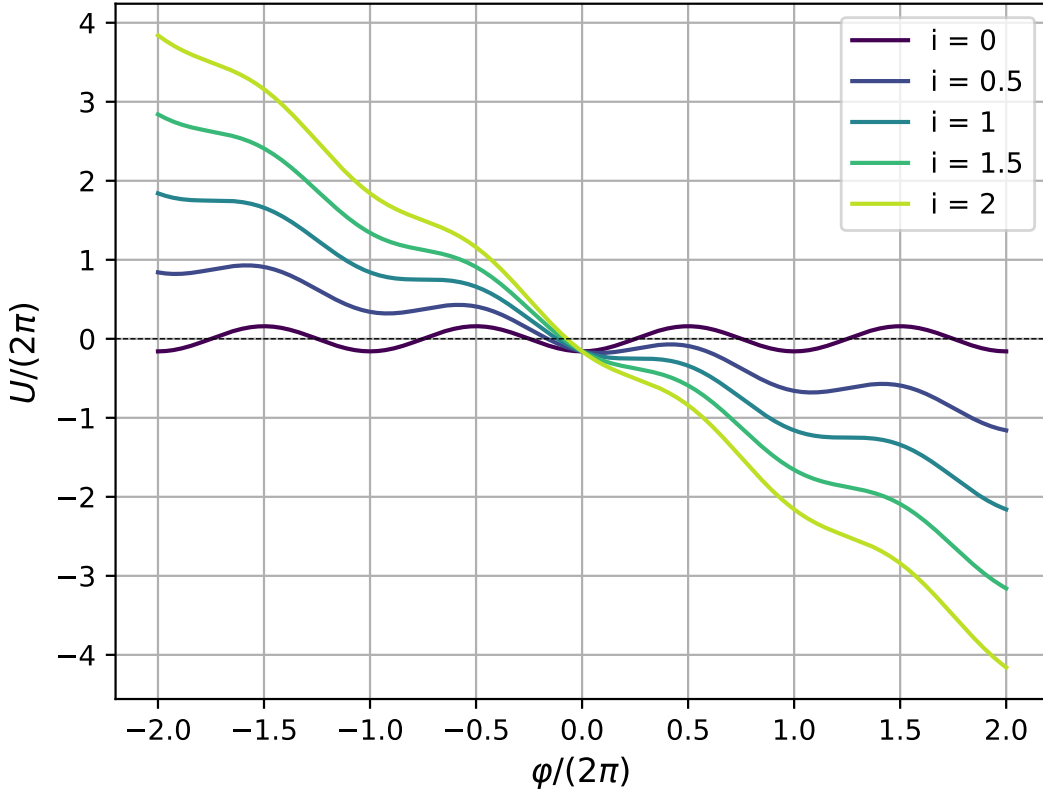


Figure 7: Tilted Washboard potential  $U(\varphi) = -i_0\varphi - \cos(\varphi)$  for different  $i$

## 6.1 Deterministic Case

The dimensionless ODE without noise reads

$$\dot{\varphi}(\tau) = i_0 - \sin(\varphi(\tau)). \quad (139)$$

### 6.1.1 Zero-Voltage State ( $i \leq 1$ )

For  $i \leq 1$ , the steady-state (SS) solution  $\varphi_{\text{SS}} = \arcsin(i_0) + 2k\pi, k \in \mathbb{Z} = \text{const}$  exists (FALSCH: NICHT 2KPI). This solution is stable:

$$\begin{aligned} \frac{d}{d\varphi} (i_0 - \sin(\varphi)) &= -\cos(\varphi) \\ -\cos(\varphi_{\text{SS}}) &= -\cos(\arcsin(i_0) + k\pi) = \pm \cos(\arcsin(i_0)) = \pm \sqrt{1 - i_0^2} \end{aligned}$$

The term  $-\sqrt{1 - i_0^2}$  is  $< 0$  for  $i_0 < 1$  (stable) and  $= 0$  for  $i_0 = 1$  (metastable). Thus, for  $i_0 < 1$ , the solution  $\varphi(\tau)$  converges to the steady-state solution  $\varphi_{\text{SS}} = \arcsin(i_0) + 2k\pi, k \in \mathbb{Z}$ .

### 6.1.2 Finite-Voltage State ( $i > 1$ )

For  $i_0 > 1$ , we can solve the ODE via separation of variables:

$$\int \frac{1}{i_0 - \sin(\varphi)} d\varphi = \int_{\tau_0}^{\tau} dt'$$

The indefinite integral on the LHS has the standard solution

$$\frac{2}{\sqrt{i_0^2 - 1}} \arctan \left( \frac{-1 + i_0 \tan(\varphi/2)}{\sqrt{i_0^2 - 1}} \right) = \tau - \tau_0$$

Rearranging:

$$\tan(\varphi/2) = \sqrt{1 - \frac{1}{i_0^2}} \tan \left( \frac{\sqrt{i_0^2 - 1}}{2} (\tau - \tau_0) \right) + \frac{1}{i_0}$$

Taking the  $\arctan()$  on both sides (note that  $\tan$  is not continuous - introduce a counter  $k(t)$  that counts the number of periods:

$$\boxed{\varphi(\tau) = 2 \arctan \left( \sqrt{1 - \frac{1}{i_0^2}} \tan \left( \frac{\sqrt{i_0^2 - 1}}{2} (\tau - \tau_0) \right) + \frac{1}{i_0} \right) + 2k(t)\pi, \quad k(t) \in \mathbb{Z}} \quad (140)$$

The difference  $\varphi(\tau + \hat{T}) - \varphi(\tau) = 2\pi$  is constant with period  $\hat{T} = 2\pi/\sqrt{i_0^2 - 1}$  (since  $\tan$  is  $\pi$ -periodic). The normalized voltage  $Vt_0/\phi_0$  can be computed via

$$\begin{aligned} Vt_0/\phi_0 &= \frac{d\varphi(\tau)}{d\tau} = \frac{i_0(i_0^2 - 1)}{\sqrt{i_0^2 - 1} \sin \left( (\tau - \tau_0) \sqrt{i_0^2 - 1} \right) + \cos \left( (\tau - \tau_0) \sqrt{i_0^2 - 1} \right) + i_0^2} \\ &= \frac{i_0 \omega_0^2}{\omega_0 \sin((\tau - \tau_0)\omega_0) + \cos((\tau - \tau_0)\omega_0) + i_0^2} \end{aligned}$$

with  $\omega_0 = \sqrt{i_0^2 - 1}$ . Using the trigonometric identity  $A \sin(x) + B \cos(x) = \sqrt{A^2 + B^2} \sin(x + \arctan(B/A))$ :

$$\frac{d\varphi(\tau)}{d\tau} = V t_0 / \phi_0 = \frac{\omega_0^2}{\sin((\tau - \tau_0)\omega_0 + \arctan(1/\omega_0)) + i_0} \quad (141)$$

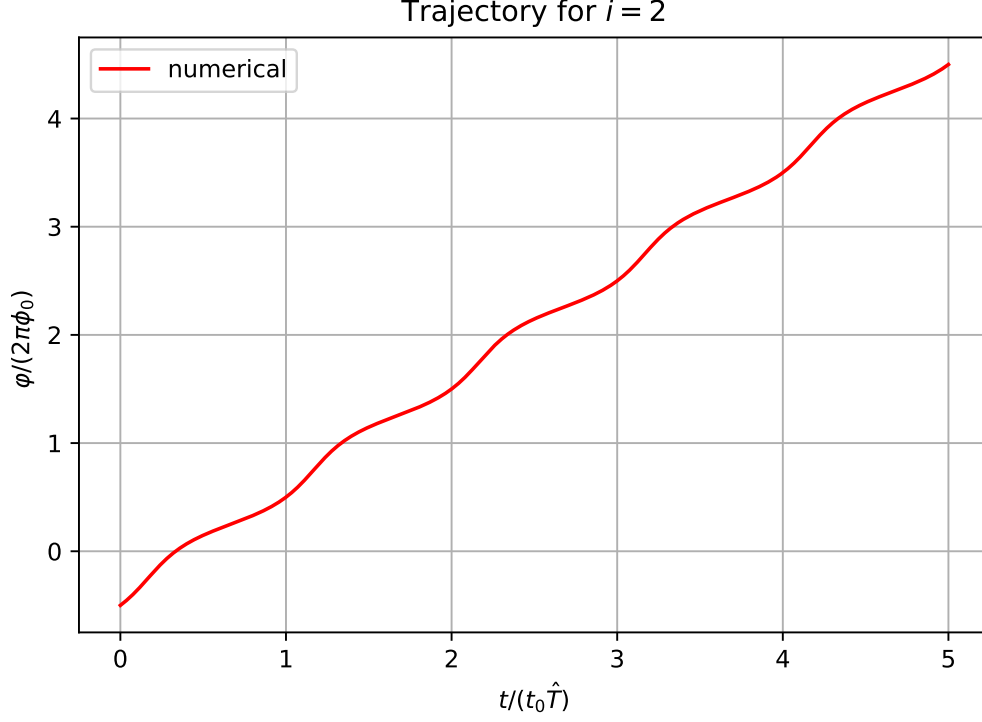


Figure 8: Node flux trajectory for  $i_0 = 2$ .  $N_t = 10^4$  time steps.  $\varphi(0) = -\pi i$  and  $T = 5\hat{T} = 10\pi/\sqrt{i^2 - 1}$

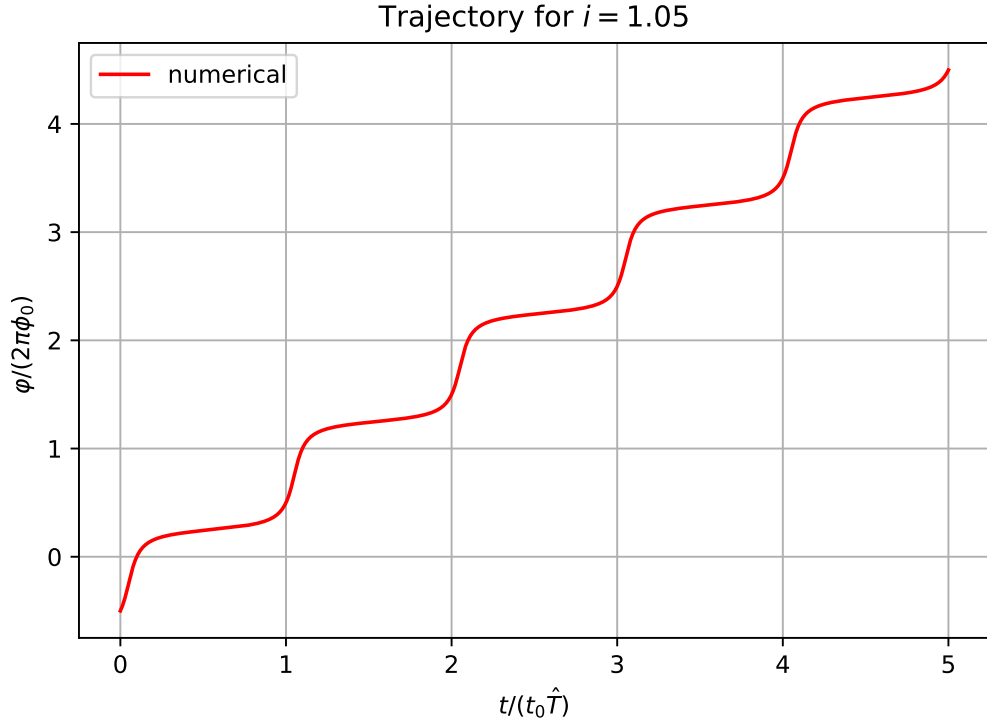


Figure 9: Node flux trajectory for  $i_0 = 1.05$ .  $N_t = 10^4$  time steps.  $\varphi(0) = -\pi$  and  $T = 5\hat{T} = 10\pi/\sqrt{i^2 - 1}$

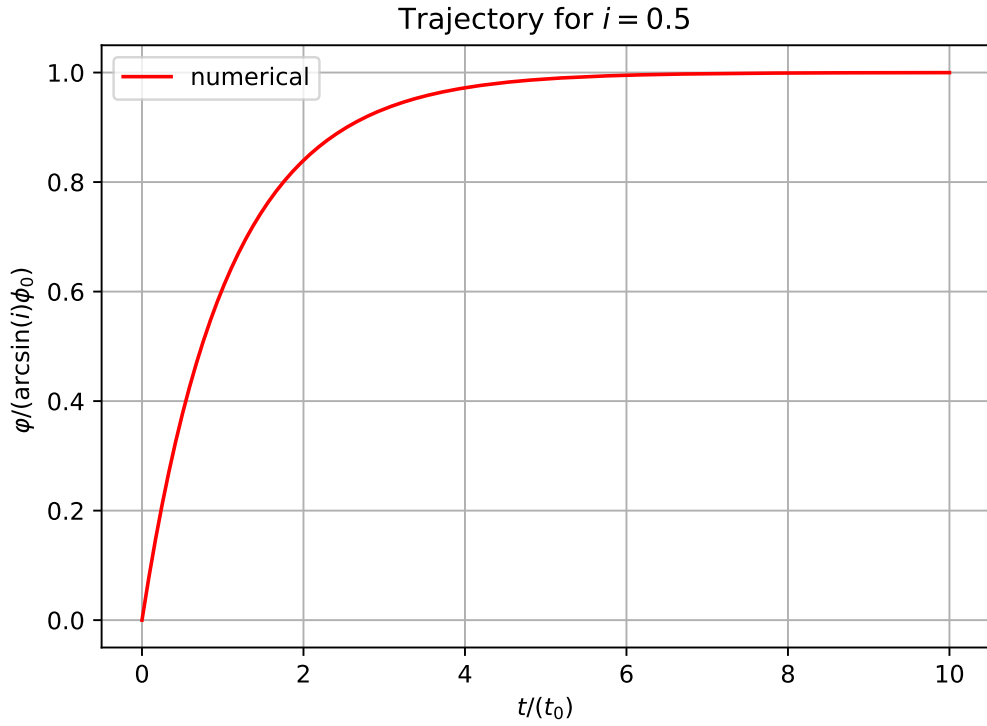


Figure 10: Node flux trajectory for  $i_0 = 0.5$ .  $N_t = 10^4$  time steps.  $\varphi(0) = 0$  and  $T = 10$

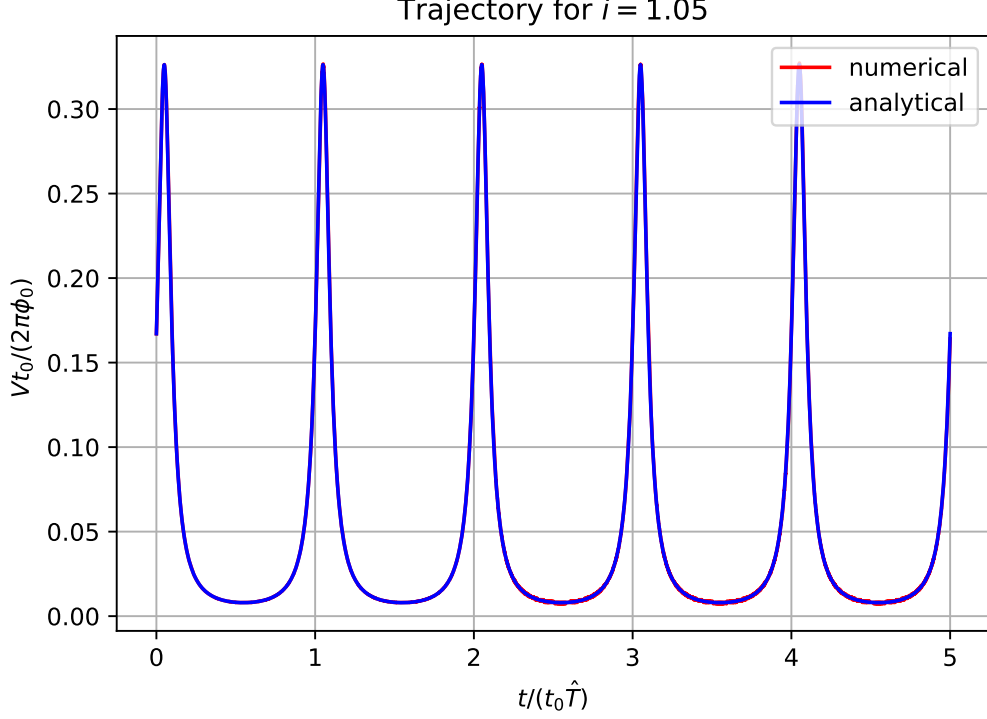


Figure 11: Voltage trajectory for  $i_0 = 1.05$ .  $N_t = 10^4$  time steps.  $\varphi(0) = -\pi$  and  $T = 10\hat{T}$ . The numerical solution was computed from the node flux via central differences

### 6.1.3 Deterministic $I - V$ Curve

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

$$\begin{aligned}\bar{V} &= \frac{1}{T} \int_{-T/2}^{T/2} V(t) dt = \frac{1}{T} (\phi(T/2) - \phi(-T/2)) = \frac{\phi_0}{\hat{T}t_0} (\varphi(\hat{T}/2) - \varphi(-\hat{T}/2)) = \frac{2\pi\phi_0}{\hat{T}t_0} \\ &= 2\pi \frac{\hbar}{2e} \frac{2eRI_c}{\hbar} \frac{\sqrt{i_0^2 - 1}}{2\pi} = RI_c \sqrt{i_0^2 - 1}\end{aligned}$$

When  $i_0 \rightarrow 1$  it follows that  $\hat{T} \rightarrow \infty$ . This yields  $\varphi(\hat{T}) = \text{const} = \arcsin(i_0)$  and thus  $\bar{V} = 0$  for  $i_0 \leq 1$ .

In summary:

$$\boxed{\frac{\bar{V}(i_0)}{RI_c} = \begin{cases} i_0 \leq 1 & 0 \\ i_0 > 1 & \sqrt{i_0^2 - 1} \end{cases}} \quad (142)$$

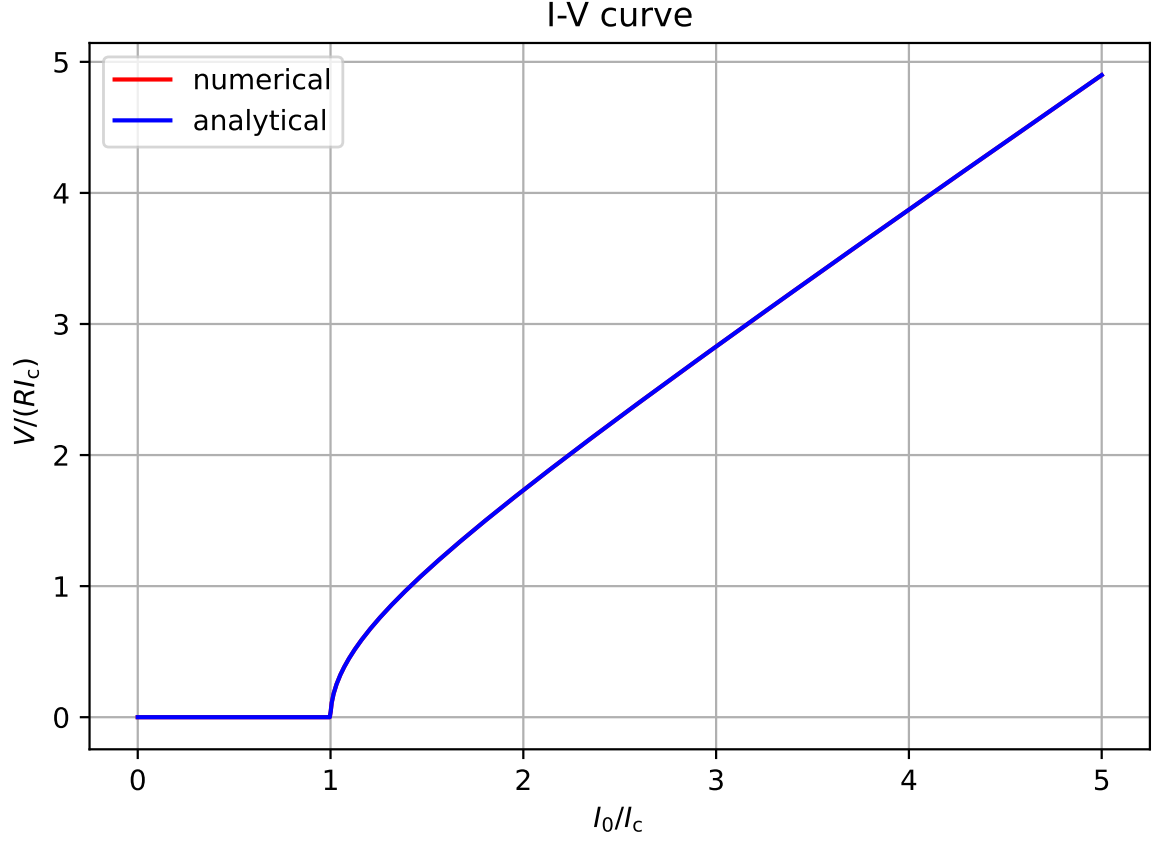


Figure 12:  $I - V$  curve of the overdamped RCSJ circuit without noise. Increments for  $i_0 : 0.005$ .  $N_t = 10^4$  time steps. For  $i_0 \leq 1$ : Starting value:  $\varphi(0) = \arcsin(i_0)$  and  $T = 10^3$ . For  $i_0 > 1$ :  $\varphi(0) = -\pi$  and  $T = \hat{T} = 2\pi/\sqrt{i_0^2 - 1}$ .

## 7 Overdamped RSJ Model (with noise): Solution Approaches via Langevin Framework

### 7.1 Variations of Constants Approach

Let  $\tau \in [\tau_0, \tau_0 + \hat{T}]$ . The dimensionless phase (node flux) for the deterministic (homogeneous) case then reads

$$\varphi_{\text{hom}}(\tau) = 2 \arctan \left( \sqrt{1 - \frac{1}{i_0^2}} \tan \left( \frac{\sqrt{i_0^2 - 1}}{2} (\tau - C) \right) + \frac{1}{i_0} \right)$$

Abbreviate the noise as  $b := \sqrt{2k_B T / E_J}$ . The noisy SDE is solvable via the method of variations of constants. Assume that the solution of the inhomogeneous equation  $\varphi(\tau, C(\tau))$  has the same form as the homogeneous solution, but with a time-dependent "constant"  $C(\tau)$ .

Calculate the LHS of the SDE via the chain rule:

$$\frac{d\varphi}{d\tau} = \frac{\partial \varphi}{\partial \tau} + \frac{\partial \varphi}{\partial C} \frac{dC}{d\tau} = i_0 - \sin(\varphi) + b\xi(\tau)$$

Since  $\varphi = \varphi(\tau, C(\tau))$  solves the homogeneous ODE with  $\partial \varphi / \partial \tau = i_0 - \sin(\varphi)$ , we are left with an ODE for  $C(\tau)$ :

$$\begin{aligned} \frac{dC}{d\tau} &= b\xi(\tau) \left( \frac{\partial \varphi}{\partial C} \right)^{-1} \\ \frac{dC}{d\tau} &= -b\xi(\tau) \frac{i_0 \left( \sqrt{1 - \frac{1}{i_0^2}} \sin \left( (\tau - C(\tau)) \sqrt{i_0^2 - 1} \right) + i_0 \right) + \cos \left( (\tau - C(\tau)) \sqrt{i_0^2 - 1} \right)}{i_0(i_0^2 - 1)} \end{aligned}$$

This doesn't lead anywhere.



## 7.2 Perturbation Approach from the RSJ deterministic solution ( $i_0 > 1$ ), no noise coupling

Introduce a perturbation  $\delta i_0$ . Let the perturbed phase be  $\varphi_0 + \varphi_1$  where  $\varphi_0$  solves the unperturbed ODE

$$\dot{\varphi}_0 + \dot{\varphi}_1 = i_0 - \sin(\varphi_0 + \varphi_1) + \delta i_0$$

Expand the sine term:

$$\dot{\varphi}_0 + \dot{\varphi}_1 = i_0 - \sin(\varphi_0) \cos(\varphi_1) - \cos(\varphi_0) \sin(\varphi_1) + \delta i_0$$

Let  $\varphi_1 \ll 1$ . Then, sine and cosine can be approximated:

$$\dot{\varphi}_0 + \dot{\varphi}_1 = i_0 - \sin(\varphi_0) \cdot 1 - \cos(\varphi_0) \varphi_1 + \delta i_0$$

We can separate this ODE into a set of two equations:

$$\begin{aligned}\dot{\varphi}_0 &= i_0 - \sin(\varphi_0) \\ \dot{\varphi}_1 &= -\cos(\varphi_0) \varphi_1 + \delta i_0\end{aligned}$$

We know that the originally derived solution for  $\varphi_0$  solves the first equation.

The second equation is linear in  $\varphi_1$ . We can obtain an expression for  $\cos(\varphi_0)$  by differentiating the first equation:

$$\begin{aligned}\ddot{\varphi}_0 &= -\cos(\varphi_0) \dot{\varphi}_0 \\ &\rightarrow -\cos(\varphi_0) = \frac{\ddot{\varphi}_0}{\dot{\varphi}_0}\end{aligned}$$

First, consider the homogeneous equation. Substituting into the homogeneous equation and rearranging:

$$\frac{1}{\varphi_1} \dot{\varphi}_1 = \frac{\ddot{\varphi}_0}{\dot{\varphi}_0}$$

The homogeneous solution can be found by separation of variables:

$$\begin{aligned}\int \frac{1}{\varphi_1} d\varphi_1 &= \int \frac{\ddot{\varphi}_0}{\dot{\varphi}_0} d\tau \\ \ln(\varphi_1) &= \ln(\dot{\varphi}_0) + C' \\ \varphi_1 &= C \dot{\varphi}_0\end{aligned}$$

with

$$\dot{\varphi}_0 = \frac{i_0(i_0^2 - 1)}{i_0 \left( \sqrt{1 - \frac{1}{i_0^2}} \sin\left(\tau \sqrt{i_0^2 - 1}\right) + i_0 \right) + \cos\left(\tau \sqrt{i_0^2 - 1}\right)}$$

The particular solution can be found via variation of constants, after which the ODE for  $C$  is found via

$$\begin{aligned}\dot{C} \dot{\varphi}_0 &= \delta i_0 \\ \rightarrow \dot{C} &= \frac{\delta i_0}{\dot{\varphi}_0} \\ &= \delta i_0 \frac{i_0 \left( \sqrt{1 - \frac{1}{i_0^2}} \sin\left(\tau \sqrt{i_0^2 - 1}\right) + i_0 \right) + \cos\left(\tau \sqrt{i_0^2 - 1}\right)}{i_0(i_0^2 - 1)} \\ &= \frac{\delta i_0}{i_0(i_0^2 - 1)} \left( i_0^2 + \sqrt{i_0^2 - 1} \sin\left(\tau \sqrt{i_0^2 - 1}\right) + \cos\left(\tau \sqrt{i_0^2 - 1}\right) \right)\end{aligned}$$

Assembling the full solution for  $\varphi_1$  from the homogeneous and the particular solution:

$$\varphi_1 = \dot{\varphi}_0 \left( \varphi_1(0) \frac{i_0^2 + 1}{i_0(i_0^2 - 1)} + \int_0^\tau \frac{\delta i_0}{\dot{\varphi}_0} d\tau' \right)$$

Let  $\varphi_1(0) = 0$ . To ensure that  $\varphi_1 \ll 1$ ,  $\varphi_1(0) = \varphi_1(\hat{T}_1)$  where  $\hat{T}_1$  is the duration for one period.

$$\varphi_1(0) = \varphi_1(\hat{T}_1) = 0 = \dot{\varphi}_0(\hat{T}_1) \int_0^{\hat{T}_1} \frac{\delta i_0}{\dot{\varphi}_0} d\tau$$

Because  $\varphi_0$  has period  $\hat{T} = 2\pi/\sqrt{i_0^2 - 1}$ ,  $\dot{\varphi}_0(\hat{T}_1) = \dot{\varphi}_0(\hat{T}) \neq 0$ .

There is no direct way to compute this integral. However, since  $\delta i_0 = \sqrt{2D}\xi(\tau)$  is Gaussian white noise,  $\langle \varphi_1 \rangle = 0$ , we can compute the variance after one period via

$$\begin{aligned} \langle \langle \varphi_1^2 \rangle \rangle &= \langle \varphi_1^2 \rangle - 0 = \int_0^{\hat{T}} \int_0^{\hat{T}} \frac{2D \langle \xi(\tau) \xi(\tau') \rangle}{\dot{\varphi}_0(\tau) \dot{\varphi}_0(\tau')} d\tau d\tau' \\ &= \int_0^{\hat{T}} \int_0^{\hat{T}} \frac{2D}{\dot{\varphi}_0^2} d\tau d\tau' \\ &= \int_0^{\hat{T}} \frac{2D}{i_0^2(i_0^2 - 1)^2} \left( i_0^2 + \sqrt{i_0^2 - 1} \sin\left(\tau \sqrt{i_0^2 - 1}\right) + \cos\left(\tau \sqrt{i_0^2 - 1}\right) \right)^2 d\tau \end{aligned}$$

With  $(a + b + c)^2 = a^2 + a(2b + 2c) + b^2 + 2bc + c^2$  and since the integral over  $\sin(x)$ ,  $\cos(x)$  and  $\sin(x) \cos(x)$  over one period is 0:

$$\begin{aligned} \langle \langle \varphi_1^2 \rangle \rangle &= \frac{2D}{i_0^2(i_0^2 - 1)^2} \int_0^{\hat{T}} \left( i_0^4 + (i_0^2 - 1) \sin^2(\tau \sqrt{i_0^2 - 1}) + \cos^2(\tau \sqrt{i_0^2 - 1}) \right) d\tau \\ &= \frac{2D}{i_0^2(i_0^2 - 1)^2} \left( i_0^4 \hat{T} + (i_0^2 - 1) \frac{\hat{T}}{2} + \frac{\hat{T}}{2} \right) \\ &= \frac{4\pi D}{(i_0^2 - 1)^{5/2}} \left( i_0^2 + \frac{1}{2} \right) \end{aligned}$$

Let  $\langle \langle \varphi_1^2 \rangle \rangle \ll 1$ , which would mean that  $|\varphi_1| \ll 1$  over one period with a high degree of certainty.

$$\begin{aligned} \langle \langle \varphi_1^2 \rangle \rangle &= \frac{4\pi D}{(i_0^2 - 1)^{5/2}} \left( i_0^2 + \frac{1}{2} \right) \ll 1 \\ &\rightarrow D \ll \frac{(i_0^2 - 1)^{5/2}}{4\pi \left( i_0^2 + \frac{1}{2} \right)} \end{aligned}$$

Because  $\varphi_1 \ll 1$ , the long-time limit remains unchanged; hence this ansatz is not suitable to determine the perturbed I-V curve.

### 7.3 Perturbation Approach from the RSJ deterministic Solution (Fourier Series Expansion) 06/06/25

Introduce a perturbation  $\sqrt{2D}\xi(\tau)$ . Let the perturbed phase be  $\varphi_0 + \varphi_1$ , where  $\varphi_0$  solves the unperturbed ODE

$$\dot{\varphi}_0 + \dot{\varphi}_1 = i_0 - \sin(\varphi_0 + \varphi_1) + \sqrt{2D}\xi(\tau)$$

Expand the sine term:

$$\dot{\varphi}_0 + \dot{\varphi}_1 = i_0 - \sin(\varphi_0)\cos(\varphi_1) - \cos(\varphi_0)\sin(\varphi_1) + \sqrt{2D}\xi(\tau)$$

Include terms up to first order for  $\varphi_1$ .

$$\dot{\varphi}_0 + \dot{\varphi}_1 = i_0 - \sin(\varphi_0) - \cos(\varphi_0)\varphi_1 + \sqrt{2D}\xi(\tau)$$

Separate the noise into slow and fast varying terms  $\xi(\tau) = \xi_{<}(\tau) + \xi_{>}(\tau)$ , where the frequency of the slow varying noise  $\xi_{<}(\tau)$  is much smaller than one period  $T = 2\pi/\sqrt{i_0^2 - 1}$ .

$$\begin{aligned}\dot{\varphi}_0 &= (i_0 + \sqrt{2D}\xi_{<}(\tau)) - \sin(\varphi_0) \\ \dot{\varphi}_1 &= -\cos(\varphi_0)\varphi_1 + \sqrt{2D}\xi_{>}(\tau)\end{aligned}$$

Assume that  $\phi_0$  is still a solution for the perturbed equation with slow varying noise. Let the solution with slow varying noise be  $\varphi_0(\tau) = \varphi_0(\tau, i_0 \rightarrow i_0 + \sqrt{2D}\xi_{<}(\tau))$

The second equation is linear in  $\varphi_1$  and separable. We can obtain an expression for  $\cos(\varphi_0)$  by differentiating the first equation:

$$\begin{aligned}\ddot{\varphi}_0 &= -\cos(\varphi_0)\dot{\varphi}_0 \\ \rightarrow -\cos(\varphi_0) &= \frac{\ddot{\varphi}_0}{\dot{\varphi}_0}\end{aligned}$$

First, consider the homogeneous equation. Substituting into the homogeneous equation and rearranging:

$$\frac{1}{\varphi_1}\dot{\varphi}_1 = \frac{\ddot{\varphi}_0}{\dot{\varphi}_0}$$

The homogeneous solution can be found by separation of variables:

$$\begin{aligned}\int \frac{1}{\varphi_1}d\varphi_1 &= \int \frac{\ddot{\varphi}_0}{\dot{\varphi}_0}d\tau \\ \ln(\varphi_1) &= \ln(\dot{\varphi}_0) + C' \\ \varphi_1 &= C\dot{\varphi}_0\end{aligned}$$

The particular solution can be found via variation of constants, after which the ODE for  $C$  is found via

$$\begin{aligned}\dot{C}\dot{\varphi}_0 &= \sqrt{2D}\xi_{>}(\tau) \\ \rightarrow \dot{C} &= \frac{\sqrt{2D}\xi_{>}(\tau)}{\dot{\varphi}_0}\end{aligned}$$

Assembling the full solution for  $\varphi_1$  from the homogeneous and the particular solution:

$$\varphi_1 = \dot{\varphi}_0 \left( C + \int_0^\tau \frac{\sqrt{2D}\xi_>(\tau')}{\dot{\varphi}_0} d\tau' \right)$$

Where  $C$  encodes the initial condition. Let this initial condition be  $\varphi_1(0) = 0$ . thus

$$\varphi_1 = \int_0^\tau \frac{\sqrt{2D}\xi_>(\tau')}{\dot{\varphi}_0} d\tau' = \int_0^\tau A(i_{\xi<}) \sin(\omega(i_{\xi<}) + \theta(i_{\xi<})) \sqrt{2D}\xi_>(\tau') d\tau'$$

The derivative of the perturbed solution is

$$\dot{\varphi}_0 + \dot{\varphi}_1 = \dot{\varphi}_0(\tau, i_{\xi<}) + \frac{\sqrt{2D}\xi_>(\tau')}{\dot{\varphi}_0(\tau, i_{\xi<})}$$

where  $i_\xi = i_0 + \sqrt{2D}\xi_<(\tau)$ . Since  $\dot{\varphi}_0(\tau, i_\xi)$  is periodic with period  $2\pi/\sqrt{(i_0 + \sqrt{2D}\xi_<(\tau))^2 - 1}$ , these terms can be expressed via a Fourier series expansion:

$$\dot{\varphi}_0 + \dot{\varphi}_1 = \sum_{k \in \mathbb{Z}} \phi_{k,0} e^{ik\tau\omega(i_{\xi<})} + \int_0^\tau A(i_{\xi<}) \sin(\omega(i_{\xi<}) + \theta(i_{\xi<})) \sqrt{2D}\xi_>(\tau') d\tau'$$

with

$$\phi_{k,0} = \frac{\omega(i_{\xi<})}{2\pi} \int_{-\pi/\omega(i_{\xi<})}^{-\pi/\omega(i_{\xi<})} \dot{\varphi}_0(\tau, i_{\xi<}) e^{-ik\tau\omega(i_{\xi<})} d\tau \quad (143)$$

and

$$\begin{aligned} \omega(i_{\xi<}) &= \sqrt{(i_0 + \sqrt{2D}\xi_<(\tau))^2 - 1} \\ &\stackrel{\text{Taylor}}{\approx} \sqrt{i_0^2 - 1} + \frac{i_0}{\sqrt{i_0^2 - 1}} \sqrt{2D}\xi_<(\tau) \\ &= \omega_0 + \frac{i_0}{\omega_0} \sqrt{2D}\xi_<(\tau), \quad \omega_0 = \sqrt{i_0^2 - 1} \end{aligned}$$

Substituting:

$$\dot{\varphi} \approx \sum_{k \in \mathbb{Z}} \phi_{k,0} e^{ik\tau\omega_0} e^{ik\tau \frac{i_0}{\omega_0} \sqrt{2D}\xi_<(\tau)} + \int_0^\tau A(i_{\xi<}) \sin(\omega(i_{\xi<}) + \theta(i_{\xi<})) \sqrt{2D}\xi_>(\tau') d\tau'$$

1. Mean:  $\langle \dot{\varphi} \rangle$ :

Take the expectation

$$\begin{aligned} \langle \dot{\varphi} \rangle &\approx \sum_{k \in \mathbb{Z}} \langle \phi_{k,0} e^{ik\tau \frac{i_0}{\omega_0} \sqrt{2D}\xi_<(\tau)} \rangle e^{ik\tau\omega_0} + \int_0^\tau A(i_\xi) \sin(\omega(i_\xi) + \theta(i_\xi)) \sqrt{2D} \langle \xi_>(\tau') \rangle d\tau' \\ &= \sum_{k \in \mathbb{Z}} \langle \phi_{k,0} e^{ik\tau \frac{i_0}{\omega_0} \sqrt{2D}\xi_<(\tau)} \rangle e^{ik\tau\omega_0} \end{aligned}$$

take the mean over one period:

$$\langle \dot{\varphi} \rangle \approx \langle \phi_{0,0} \rangle \approx \frac{\omega_0}{2\pi} \left( \int_{-\pi/\omega_0}^{-\pi/\omega_0} \dot{\varphi}_0(\tau, i_0) d\tau \right) = \omega_0 = \sqrt{i_0^2 - 1}$$

2. Variance  $\langle \langle \varphi^2 \rangle \rangle$ :

## 7.4 Perturbation Approach: Modified Time ( $i_0 > 1$ ) + Picard Iteration

Consider the ansatz  $\varphi(\tau) = \varphi_0(\tau + \theta(\tau)/\omega_0)$  where  $\omega_0 = \sqrt{i_0^2 - 1}$ . Substitute into the RSJ model equations:

$$\dot{\varphi} = \left(1 + \frac{\dot{\theta}}{\omega_0}\right)\dot{\varphi}_0 = i_0 - \sin(\varphi_0) + \sqrt{2D}\xi(\tau)$$

Separate the noise-free system and the perturbation:

$$\begin{aligned}\dot{\varphi}_0\left(\tau + \frac{\theta}{\omega_0}\right) &= i_0 - \sin\left(\varphi_0\left(\tau + \frac{\theta}{\omega_0}\right)\right) \\ \frac{\dot{\theta}}{\omega_0}\dot{\varphi}_0 &= \sqrt{2D}\xi(\tau)\end{aligned}$$

Rearranging:

$$\begin{aligned}\dot{\varphi}_0 &= i_0 - \sin(\varphi_0) \\ \dot{\theta} &= \frac{\omega_0}{\dot{\varphi}_0}\sqrt{2D}\xi(\tau)\end{aligned}$$

The first equation has the analytical solution as derived earlier (see [Equation 140](#), with the substitution  $\tau \rightarrow \tau + \theta/\omega_0$ ). The term  $\omega_0/\dot{\varphi}_0$  is known (see [Equation 141](#)):

$$\frac{\omega_0}{\dot{\varphi}_0} = \frac{1}{\omega_0} [\sin(\tau\omega_0 + \theta + \arctan(1/\omega_0)) + i_0]$$

Substitute  $\arctan(1/\omega_0) = \Delta\theta_0$ . The SDE for  $\theta$  becomes:

$$\dot{\theta} = \frac{1}{\omega_0} [\sin(\tau\omega_0 + \theta + \Delta\theta_0) + i_0] \sqrt{2D}\xi(\tau)$$

We are interested in the term  $\langle \bar{\dot{\varphi}} \rangle = \overline{\langle (1 + \dot{\theta}/\omega_0)\dot{\varphi}_0 \rangle} = \langle \bar{\dot{\varphi}_0} \rangle + \langle \bar{\dot{\theta}}\bar{\dot{\varphi}_0} \rangle/\omega_0$ . Assume that  $\theta$  changes slowly compared to  $\varphi$ . Then,  $\langle \dot{\theta}\dot{\varphi}_0 \rangle = \text{Cov}(\dot{\theta}, \dot{\varphi}_0) + \langle \dot{\theta} \rangle \langle \dot{\varphi}_0 \rangle \approx \langle \dot{\theta} \rangle \langle \dot{\varphi}_0 \rangle \approx \langle \dot{\theta} \rangle \dot{\varphi}_0$ . All that remains is determining  $\langle \dot{\theta} \rangle$ .

The variance  $\text{Var}(\varphi(\tau + \theta/\omega_0))$ :

$$\begin{aligned}\text{Var}(\varphi(\tau + \theta/\omega_0)) &= (\varphi'(\tau + \langle \theta(\tau) \rangle/\omega_0))^2 \text{Var}(\theta(\tau)) \\ &= \left( \frac{\omega_0^2}{\sin((\tau + \langle \theta(\tau) \rangle/\omega_0)\omega_0) + \arctan(1/\omega_0) + i_0} \right)^2 \text{Var}(\theta(\tau))\end{aligned}$$

**Picard iteration method states:**

Consider the initial value problem  $\theta(\tau) = f(\tau, \theta(\tau))$ ,  $\theta(0) = \theta_0$  where  $f(\theta(\tau), \tau)$  is continuous and Lipschitz continuous in the second argument  $\theta$ . The series  $\theta_n(\tau)$ ,  $\tau \in [0, \epsilon]$  converges uniformly towards the exact solution  $\theta(\tau)$  for sufficiently small  $\epsilon$ . The series  $\theta_n$  is given by:

$$\begin{aligned}\theta_0(\tau) &= \theta_0 \\ \theta_{n+1}(\tau) &= \theta_0 + \int_0^\tau f(t, \theta_n(t)) dt\end{aligned}$$

From this, we determine the derivative  $\dot{\theta}$ :

$$\begin{aligned}\dot{\theta}_0(\tau) &= 0 \\ \dot{\theta}_{n+1}(\tau) &= f(\tau, \theta_n(\tau))\end{aligned}$$

Apply the Picard iteration method for solving the SDE in  $\tau$ . Let  $\theta(0) = 0$ . Then,

$$\begin{aligned}\theta_0(\tau) &= 0 \\ \theta_1(\tau) &= \int_0^\tau \frac{1}{\omega_0} [\sin(\omega_0 t + \Delta\theta_0) + i_0] \sqrt{2D} \xi(t) dt \\ \theta_2(\tau) &= \int_0^\tau \frac{1}{\omega_0} \left[ \sin \left( \omega_0 t + \Delta\theta_0 + \int_0^t \frac{1}{\omega_0} [\sin(\omega_0 t' + \Delta\theta_0) + i_0] \sqrt{2D} \xi(t') dt' \right) + i_0 \right] \sqrt{2D} \xi(t) dt \\ &\dots \\ \theta_{n+1}(\tau) &= \int_0^\tau \frac{1}{\omega_0} [\sin(\omega_0 t + \Delta\theta_0 + \theta_n(t)) + i_0] \sqrt{2D} \xi(t) dt\end{aligned}$$

and for the derivatives:

$$\begin{aligned}\dot{\theta}_0(\tau) &= 0 \\ \dot{\theta}_1(\tau) &= \frac{1}{\omega_0} [\sin(\omega_0 \tau + \Delta\theta_0) + i_0] \sqrt{2D} \xi(\tau) \\ \dot{\theta}_2(\tau) &= \frac{1}{\omega_0} \left[ \sin \left( \omega_0 \tau + \Delta\theta_0 + \int_0^\tau \frac{1}{\omega_0} [\sin(\omega_0 t + \Delta\theta_0) + i_0] \sqrt{2D} \xi(t) dt \right) + i_0 \right] \sqrt{2D} \xi(\tau) \\ &\dots \\ \dot{\theta}_{n+1}(\tau) &= \frac{1}{\omega_0} [\sin(\omega_0 \tau + \Delta\theta_0 + \theta_n(\tau)) + i_0] \sqrt{2D} \xi(\tau)\end{aligned}$$

Taking expectation of the derivative:

$$\begin{aligned}\langle \dot{\theta}_{n+1}(\tau) \rangle &= \left\langle \frac{1}{\omega_0} [\sin(\omega_0 \tau + \Delta\theta_0 + \theta_n(\tau)) + i_0] \sqrt{2D} \xi(\tau) \right\rangle \\ &= \left\langle \frac{1}{\omega_0} \sin(\omega_0 \tau + \Delta\theta_0 + \theta_n(\tau)) \sqrt{2D} \xi(\tau) \right\rangle \\ &= \frac{1}{\omega_0} \sin(\omega_0 \tau + \Delta\theta_0) \left\langle \cos(\theta_n(\tau)) \sqrt{2D} \xi(\tau) \right\rangle + \frac{1}{\omega_0} \cos(\omega_0 \tau + \Delta\theta_0) \left\langle \sin(\theta_n(\tau)) \sqrt{2D} \xi(\tau) \right\rangle\end{aligned}$$

Now calculate the first couple  $\langle \dot{\theta}_n(\tau) \rangle$  :

For  $\theta_1(\tau)$ :

$$\begin{aligned}\langle \dot{\theta}_1(\tau) \rangle &= \frac{1}{\omega_0} \sin(\omega_0\tau + \Delta\theta_0) \langle \cos(0)\sqrt{2D}\xi(\tau) \rangle + \frac{1}{\omega_0} \cos(\omega_0\tau + \Delta\theta_0) \langle \sin(0)\sqrt{2D}\xi(\tau) \rangle \\ &= \frac{1}{\omega_0} \sin(\omega_0\tau + \Delta\theta_0) \langle \sqrt{2D}\xi(\tau) \rangle = 0\end{aligned}$$

This is expected, since  $\theta_1(\tau)$  is a stochastic integral of Brownian motion  $\rightarrow \theta_1(\tau)$  is Gaussian (colored) noise, since the integral is linear and  $\xi(\tau)$  is Gaussian with  $\theta_1(\tau) \sim \mathcal{N}(0, \text{Var}(\theta_1(\tau)))$ . Calculate  $\text{Var}(\theta_1)$ : Using  $\xi(t)dt = dw(t)$  and  $dw(t)dw(t') \neq 0$  only when  $t = t'$

$$\begin{aligned}\langle \theta_1^2(\tau) \rangle &= \text{Var}(\theta_1)(\tau) = \left\langle \int_0^\tau \int_0^\tau \frac{2D}{\omega_0^2} [\sin(\omega_0 t + \Delta\theta_0) + i_0] [\sin(\omega_0 t' + \Delta\theta_0) + i_0] dw(t)dw(t') \right\rangle \\ &= \int_0^\tau \frac{2D}{\omega_0^2} [\sin(\omega_0 t + \Delta\theta_0) + i_0]^2 dt \\ &= \frac{2D}{\omega_0^2} \int_0^\tau (\sin^2(\omega_0 t + \Delta\theta_0) + 2i_0 \sin(\omega_0 t + \Delta\theta_0) + i_0^2) dt \\ &= \frac{2D}{\omega_0^2} \left( \frac{2\omega_0\tau + \sin(2\Delta\theta_0) - \sin(2(\omega_0\tau + \Delta\theta_0))}{4\omega_0} + 2i_0 \frac{\cos(\Delta\theta_0) - \cos(\omega_0\tau + \Delta\theta_0)}{\omega_0} + i_0^2\tau \right) \\ &= \frac{2D}{\omega_0^2} \left( \frac{\sin(2\Delta\theta_0) - \sin(2(\omega_0\tau + \Delta\theta_0))}{4\omega_0} + 2i_0 \frac{\cos(\Delta\theta_0) - \cos(\omega_0\tau + \Delta\theta_0)}{\omega_0} + (i_0^2 + \frac{1}{2})\tau \right)\end{aligned}$$

For  $\theta_2(\tau)$ :

$$\begin{aligned}\langle \dot{\theta}_2(\tau) \rangle &= \frac{1}{\omega_0} \sin(\omega_0\tau + \Delta\theta_0) \langle \cos(\theta_1(\tau))\sqrt{2D}\xi(\tau) \rangle + \frac{1}{\omega_0} \cos(\omega_0\tau + \Delta\theta_0) \langle \sin(\theta_1(\tau))\sqrt{2D}\xi(\tau) \rangle \\ &= \frac{\sqrt{2D}}{\omega_0} [\sin(\omega_0\tau + \Delta\theta_0) \langle \cos(\theta_1(\tau))\xi(\tau) \rangle + \cos(\omega_0\tau + \Delta\theta_0) \langle \sin(\theta_1(\tau))\xi(\tau) \rangle]\end{aligned}$$

Calculate the expectations: These terms have the shape  $\langle f(\xi(\tau))\xi(\tau) \rangle$ . For an arbitrary function  $f$  and Gaussian noise  $\xi(\tau) \sim \mathcal{N}(0, 1^2)$  this term can be expressed as:

$$\begin{aligned}\langle f(\xi(\tau))\xi(\tau) \rangle &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)x \exp\left(-\frac{x^2}{2}\right) dx \\ &= -\frac{1}{\sqrt{2\pi}} f(x) \exp\left(-\frac{x^2}{2}\right) \Big|_{-\infty}^{\infty} + \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{df(x)}{dx} \exp\left(-\frac{x^2}{2}\right) dx \\ &= 0 + \left\langle \frac{df(\xi(\tau))}{d\xi(\tau)} \right\rangle\end{aligned}$$

Applying this to the term  $\langle \dot{\theta}_2(\tau) \rangle$  yields:

$$\begin{aligned}\langle \dot{\theta}_2(\tau) \rangle &= \frac{\sqrt{2D}}{\omega_0} \left[ \sin(\omega_0\tau + \Delta\theta_0) \left\langle \frac{d \cos(\theta_1(\tau))}{d\xi(\tau)} \right\rangle + \cos(\omega_0\tau + \Delta\theta_0) \left\langle \frac{d \sin(\theta_1(\tau))}{d\xi(\tau)} \right\rangle \right] \\ &= \frac{\sqrt{2D}}{\omega_0} \left[ -\sin(\omega_0\tau + \Delta\theta_0) \left\langle \frac{d\theta_1(\tau)}{d\xi(\tau)} \sin(\theta_1(\tau)) \right\rangle + \cos(\omega_0\tau + \Delta\theta_0) \left\langle \frac{d\theta_1(\tau)}{d\xi(\tau)} \cos(\theta_1(\tau)) \right\rangle \right]\end{aligned}$$

It is straightforward to calculate  $d\theta_1(\tau)/d\xi(\tau)$

$$\frac{d\theta_1(\tau)}{d\xi(\tau)} = \frac{1}{\omega_0} [\sin(\omega_0\tau + \Delta\theta_0) + i_0] \sqrt{2D}$$

Substituting back:

$$\begin{aligned} \langle \dot{\theta}_2(\tau) \rangle = \frac{2D}{\omega_0^2} [\sin(\omega_0\tau + \Delta\theta_0) + i_0] & \left( -\sin(\omega_0\tau + \Delta\theta_0) \langle \sin(\theta_1(\tau)) \rangle \right. \\ & \left. + \cos(\omega_0\tau + \Delta\theta_0) \langle \cos(\theta_1(\tau)) \rangle \right) \end{aligned}$$

Now calculate  $\langle \sin(\theta_1(\tau)) \rangle$  and  $\langle \cos(\theta_1(\tau)) \rangle$ . Both can be expressed as:

$$\begin{aligned} \langle \sin(\theta_1(\tau)) \rangle &= \left\langle \text{Im}(e^{i\theta_1(\tau)}) \right\rangle = \text{Im} \left\{ \frac{1}{\sqrt{2\pi \text{Var}(\theta_1)}} \int_{-\infty}^{\infty} e^{i\theta_1} \exp\left(-\frac{\theta_1^2}{2\text{Var}(\theta_1)}\right) d\theta_1 \right\} \\ &= \text{Im} \left\{ \exp\left(-\frac{1}{2}\text{Var}(\theta_1)\right) \right\} = 0 \\ \langle \cos(\theta_1(\tau)) \rangle &= \left\langle \text{Re}(e^{i\theta_1(\tau)}) \right\rangle = \text{Re} \left\{ \frac{1}{\sqrt{2\pi \text{Var}(\theta_1)}} \int_{-\infty}^{\infty} e^{i\theta_1} \exp\left(-\frac{\theta_1^2}{2\text{Var}(\theta_1)}\right) d\theta_1 \right\} \\ &= \exp\left(-\frac{1}{2}\text{Var}(\theta_1)\right) \end{aligned}$$

which could have also been calculated via the characteristic function. This would mean that  $\langle \dot{\theta}_2(\tau) \rangle \rightarrow 0$  for  $\tau \rightarrow \infty$ . Assembling everything:

$$\begin{aligned} \langle \dot{\theta}_2(\tau) \rangle &= \frac{2D}{\omega_0^2} [\sin(\omega_0\tau + \Delta\theta_0) + i_0] \cos(\omega_0\tau + \Delta\theta_0) \\ &\quad \exp\left(-\frac{1}{2} \frac{2D}{\omega_0^2} \left( \frac{\sin(2\Delta\theta_0) - \sin(2(\omega_0\tau + \Delta\theta_0))}{4\omega_0} + 2i_0 \frac{\cos(\Delta\theta_0) - \cos(\omega_0\tau + \Delta\theta_0)}{\omega_0} + (i_0^2 + \frac{1}{2})\tau \right)\right) \end{aligned}$$



This result is also obtained using the identity  $\mathbb{E}[Xg(Y)] = \text{Cov}(X, Y)\mathbb{E}[Yg(Y)]/\sigma_Y^2$  where  $X$  and  $Y$  are jointly Gaussian variables:

$$\begin{aligned}\langle \sin(\theta_1(\tau))\xi(\tau) \rangle &= \frac{\text{Cov}(\xi(\tau), \theta_1(\tau))\langle \sin(\theta_1(\tau))\theta_1(\tau) \rangle}{\text{Var}(\theta_1(\tau))} \\ \langle \cos(\theta_1(\tau))\xi(\tau) \rangle &= \frac{\text{Cov}(\xi(\tau), \theta_1(\tau))\langle \cos(\theta_1(\tau))\theta_1(\tau) \rangle}{\text{Var}(\theta_1(\tau))}\end{aligned}$$

The characteristic function  $\langle e^{itX} \rangle$  of a normally distributed variable  $X \sim \mathcal{N}(\mu, \sigma^2)$  is equal to

$$\langle e^{itX} \rangle = e^{it\mu - \frac{1}{2}t^2\sigma^2}$$

By means of the characteristic function, we obtain

$$\langle X e^{iX} \rangle = \left. \frac{1}{i} \frac{d}{dt} \langle e^{itX} \rangle \right|_{t=1} = (\mu + i\sigma^2) e^{i\mu - \frac{1}{2}\sigma^2}$$

and therefore

$$\langle \sin(\theta_1(\tau))\theta_1(\tau) \rangle = \text{Im} \left\{ \langle \theta_1(\tau) e^{i\theta_1(\tau)} \rangle \right\} = \text{Im} \left\{ i \text{Var}(\theta_1(\tau)) \exp\left(-\frac{1}{2} \text{Var}(\theta_1(\tau))\right) \right\} \quad (144)$$

$$= \text{Var}(\theta_1(\tau)) \exp\left(-\frac{1}{2} \text{Var}(\theta_1(\tau))\right) \quad (145)$$

$$\langle \cos(\theta_1(\tau))\theta_1(\tau) \rangle = \text{Re} \left\{ \langle \theta_1(\tau) e^{i\theta_1(\tau)} \rangle \right\} = \text{Re} \left\{ i \text{Var}(\theta_1(\tau)) \exp\left(-\frac{1}{2} \text{Var}(\theta_1(\tau))\right) \right\} \quad (146)$$

$$= 0 \quad \rightarrow \quad \langle \cos(\theta_1(\tau))\xi(\tau) \rangle = 0 \quad (147)$$

Next, the covariance:

$$\begin{aligned}\text{Cov}(\xi(\tau), \theta_1(\tau)) &= \langle \xi(\tau)\theta_1(\tau) \rangle - \langle \xi(\tau) \rangle \langle \theta_1(\tau) \rangle \\ &= \left\langle \xi(\tau) \int_0^\tau \frac{1}{\omega_0} [\sin(\omega_0 t + \Delta\theta_0) + i_0] \sqrt{2D} \xi(t) dt \right\rangle - 0 \\ &= \int_0^\tau \frac{1}{\omega_0} [\sin(\omega_0 t + \Delta\theta_0) + i_0] \sqrt{2D} \underbrace{\langle \xi(\tau)\xi(t) \rangle}_{=\delta(t-\tau)} dt = \frac{1}{\omega_0} [\sin(\omega_0\tau + \Delta\theta_0) + i_0] \sqrt{2D}\end{aligned}$$

Assembling all terms together yields:

$$\begin{aligned}\langle \dot{\theta}_2(\tau) \rangle &= \frac{\sqrt{2D}}{\omega_0} \left[ \sin(\omega_0\tau + \Delta\theta_0) \underbrace{\langle \cos(\theta_1(\tau))\xi(\tau) \rangle}_{=0} + \cos(\omega_0\tau + \Delta\theta_0) \langle \sin(\theta_1(\tau))\xi(\tau) \rangle \right] \\ &= \frac{\sqrt{2D}}{\omega_0} \cos(\omega_0\tau + \Delta\theta_0) \frac{\text{Cov}(\xi(\tau), \theta_1(\tau))\langle \sin(\theta_1(\tau))\theta_1(\tau) \rangle}{\text{Var}(\theta_1(\tau))} \\ &= \frac{\sqrt{2D}}{\omega_0} \cos(\omega_0\tau + \Delta\theta_0) \frac{1}{\omega_0} [\sin(\omega_0\tau + \Delta\theta_0) + i_0] \sqrt{2D} \frac{\text{Var}(\theta_1(\tau)) \exp(-\frac{1}{2} \text{Var}(\theta_1(\tau)))}{\text{Var}(\theta_1(\tau))} \\ &= \frac{2D}{\omega_0^2} \cos(\omega_0\tau + \Delta\theta_0) [\sin(\omega_0\tau + \Delta\theta_0) + i_0] \\ &\quad \exp\left(-\frac{1}{2} \frac{2D}{\omega_0^2} \left( \frac{\sin(2\Delta\theta_0) - \sin(2(\omega_0\tau + \Delta\theta_0))}{4\omega_0} + 2i_0 \frac{\cos(\Delta\theta_0) - \cos(\omega_0\tau + \Delta\theta_0)}{\omega_0} + (i_0^2 + \frac{1}{2})\tau \right)\right)\end{aligned}$$

$$\begin{aligned}
\langle\langle\theta_2^2(\tau)\rangle\rangle &= \text{Var}(\theta_2)(\tau) = \left\langle \left( \int_0^\tau \frac{1}{\omega_0} [\sin(\omega_0 t + \Delta\theta_0 + \theta_1(\tau)) + i_0] \sqrt{2D} \xi(t) dt \right)^2 \right\rangle \\
&= \int_0^\tau \frac{2D}{\omega_0^2} \langle [\sin(\omega_0 t + \Delta\theta_0 + \theta_1(\tau)) + i_0]^2 \rangle dt \\
&= \frac{2Di_0^2}{\omega_0^2} \tau + \int_0^\tau \frac{2D}{\omega_0^2} \langle \sin^2(\omega_0 t + \Delta\theta_0 + \theta_1(\tau)) + 2i_0 \sin(\omega_0 t + \Delta\theta_0 + \theta_1(\tau)) \rangle dt
\end{aligned}$$

Using the identity  $\sin^2(x) = (1 - \cos(2x))/2$ :

$$\langle\langle\theta_2^2(\tau)\rangle\rangle = \frac{2D}{\omega_0^2} \left( i_0^2 + \frac{1}{2} \right) \tau + \int_0^\tau \frac{D}{\omega_0^2} \langle i_0 \sin(\omega_0 t + \Delta\theta_0 + \theta_1(\tau)) - \cos(2(\omega_0 t + \Delta\theta_0 + \theta_1(\tau))) \rangle dt$$

The expectations of the oscillatory terms again can be computed using the characteristic function.

## 8 Overdamped RSJ Model (with noise): Solution Approaches via Fokker-Planck Framework

### 8.1 Theory

#### 8.1.1 Wrapped Process

Decompose the process  $\varphi(\tau)$  into the sum of a counting variable  $N(\tau)$  and the process  $\theta(\tau) \in [0, 2\pi)$  on the unit circle  $\mathbb{S}^1$  ( $\theta(\tau) = \varphi(\tau) \bmod 2\pi$ ):

$$\varphi(\tau) = 2\pi N(\tau) + \theta(\tau)$$

The counter can be expressed as:

$$N(\tau) = \max\{n | T_n \leq \tau\}$$

where  $T_0 = 0, \quad T_n = \Delta T_1 + \Delta T_2 + \cdots + \Delta T_n$

where  $\Delta T_n$  is the (non-negative) first-passage time to go from  $\varphi = 2(n-1)\pi$  to  $\varphi = 2n\pi$  defined as

$$\Delta T_n = \inf\{\tau \geq 0 | \varphi(\tau) = 2n\pi\} - \inf\{\tau \geq 0 | \varphi(\tau) = 2(n-1)\pi\}$$

Since the driving force  $i_0 - \sin(\varphi(\tau))$  is periodic in  $\varphi(\tau)$ , the  $\Delta T_n$  are independent, identically distributed variables.

The counter  $N$  and  $\theta$  are connected such that  $N(\tau)$  jumps by 1 when  $\theta(\tau)$  jumps from  $2\pi$  back to 0. Note that  $\theta$  is not necessarily periodic (because of the noise term).

$N(\tau)$  and  $\theta(\tau)$  are uncorrelated except for  $\tau = T_n$ . Therefore, their variances are additive. In the long time limit:

$$\lim_{\tau \rightarrow \infty} \frac{\langle \varphi(\tau) \rangle}{\tau} = \lim_{\tau \rightarrow \infty} \left[ \frac{2\pi \langle N(\tau) \rangle}{\tau} + \frac{\langle \theta(\tau) \rangle}{\tau} \right] = \lim_{\tau \rightarrow \infty} \frac{2\pi \langle N(\tau) \rangle}{\tau} \quad (148)$$

$$\lim_{\tau \rightarrow \infty} \frac{\langle \langle \varphi^2(\tau) \rangle \rangle}{\tau} = \lim_{t \rightarrow \infty} \left[ (2\pi)^2 \frac{\langle \langle N^2(\tau) \rangle \rangle}{\tau} + \frac{\langle \langle \theta^2(\tau) \rangle \rangle}{\tau} \right] = \lim_{\tau \rightarrow \infty} (2\pi)^2 \frac{\langle \langle N^2(\tau) \rangle \rangle}{\tau} \quad (149)$$

#### 8.1.2 Renewal Theory CLT

According to reference [2] section 10.2, a renewal process  $N(\tau)$  is a process such that

$$N(\tau) = \max\{n | T_n \leq \tau\}$$

where  $T_0 = 0, \quad T_n = \Delta T_1 + \Delta T_2 + \cdots + \Delta T_n$

where  $T_0 = 0, \quad T_n = \Delta T_1 + \Delta T_2 + \cdots + \Delta T_n$  for  $n \geq 1$  and  $\{\Delta T_n\}$  is a sequence of independent, identically distributed, non-negative random variables with  $\langle \Delta T_n \rangle = \mu, \langle \langle \Delta T_n^2 \rangle \rangle = \sigma^2$ .

Then the renewal theory central limit theorem states:

$$\frac{N(\tau)}{\tau} \xrightarrow{\text{a.s.}} \frac{1}{\mu} \quad \text{as } \tau \rightarrow \infty$$

$$\frac{N(\tau) - \tau/\mu}{\sqrt{\tau\sigma^2/\mu^3}} \xrightarrow{\text{dist}} \mathcal{N}(0, 1) \quad \text{as } \tau \rightarrow \infty$$

Applying the renewal theory CLT to [Equation 149](#) yields:

$$\lim_{\tau \rightarrow \infty} \frac{\langle \varphi(\tau) \rangle}{\tau} = \lim_{\tau \rightarrow \infty} \frac{2\pi \langle N(\tau) \rangle}{\tau} = \frac{2\pi}{\mu} \quad (150)$$

$$\lim_{\tau \rightarrow \infty} \frac{\langle \langle \varphi^2(\tau) \rangle \rangle}{\tau} = \lim_{\tau \rightarrow \infty} (2\pi)^2 \frac{\langle \langle N^2(\tau) \rangle \rangle}{\tau} = (2\pi)^2 \frac{\sigma^2}{\mu^3} \quad (151)$$

This leaves only the mean  $\langle \Delta T_n \rangle = \mu$  and the variance  $\langle \langle \Delta T_n^2 \rangle \rangle = \sigma^2$  of the first passage time to be determined.

One can also show that the mean first passage time is directly related to  $j_{ss}$ , which is the stationary state probability current of the process on the circle  $\theta$ :

$$\langle \Delta T_n \rangle = \frac{2\pi}{j_{ss}}$$

This is proven in the next section:

### 8.1.3 Average Velocity and Probability Current on the Circle (Calculation of $j_{ss}$ in the next section)

Consider a stochastic process  $x(t) \in [0, L)$  on the circle governed by the SDE

$$dx(t) = F(x(t)) dt + \sqrt{2D} dW(t),$$

where  $F(x+L) = F(x)$  is periodic. Let  $X(t) \in \mathbb{R}$  be the lifted process, defined via

$$X(t) = x(t) + n(t)L,$$

where  $n(t) \in \mathbb{Z}$  counts the number of windings. Denote by  $P(X, t)$  the probability density of the lifted process on  $\mathbb{R}$ , and by  $\tilde{P}(x, t)$  the probability density on the circle  $x \in [0, L)$ . The two are related by

$$\tilde{P}(x, t) = \sum_{n \in \mathbb{Z}} P(x + nL, t).$$

The wrapped process  $\tilde{P}(x, t)$  on the circle must account for all periodically shifted probabilities  $P(x + nL, t)$

We compute the time derivative of the expected value  $\mathbb{E}[X(t)]$  using the Fokker–Planck equation. The density  $P(X, t)$  satisfies

$$\partial_t P(X, t) = -\partial_X J(X, t),$$

where the probability current is given by

$$J(X, t) = F(X) \cdot P(X, t) - D \cdot \partial_X P(X, t).$$

We compute:

$$\begin{aligned}
\frac{d}{dt}\mathbb{E}[X(t)] &= \frac{d}{dt} \int_{\mathbb{R}} X \cdot P(X, t) dX \\
&= \int_{\mathbb{R}} X \cdot \partial_t P(X, t) dX \\
&= - \int_{\mathbb{R}} X \cdot \partial_X J(X, t) dX \\
&= \int_{\mathbb{R}} J(X, t) dX \quad (\text{by integration by parts}) \\
&= \sum_{n \in \mathbb{Z}} \int_{nL}^{(n+1)L} J(X, t) dX \\
&= \sum_{n \in \mathbb{Z}} \int_0^L [F(x) \cdot P(x + nL, t) - D \cdot \partial_x P(x + nL, t)] dx \\
&= \int_0^L \left[ F(x) \cdot \sum_n P(x + nL, t) - D \cdot \partial_x \sum_n P(x + nL, t) \right] dx \\
&= \int_0^L [F(x) \cdot \tilde{P}(x, t) - D \cdot \partial_x \tilde{P}(x, t)] dx \\
&= \int_0^L \tilde{J}(x, t) dx.
\end{aligned}$$

This leads to the conclusion that:

$$\frac{d}{dt}\mathbb{E}[X(t)] = \int_0^L \tilde{J}(x, t) dx$$

In the long-time limit, the system reaches a steady state in which the current  $\tilde{J}(x, t)$  becomes constant in space and time:

$$\tilde{J}(x, t) \rightarrow J_{\text{ss}}.$$

$$\frac{d}{dt}\mathbb{E}[X(t)] \rightarrow LJ_{\text{ss}}$$

## 8.2 Approach via Probability Current of the Wrapped Process (look up Green-Kubo formula and Lifson-Jackson formula)

For  $i_0 = 0$ , the tilted washboard potential is symmetric with  $U(\varphi + 2\pi) = U(\varphi)$ . Since the noise is white noise, it favors no direction, and the PDF spreads symmetrically around the starting value. The solution has been derived in the previous section.

For  $i_0 > 0$ , the tilted washboard potential becomes tilted, with  $U(\varphi + 2\pi) - U(\varphi) = -2\pi i_0$ . Since the noise favors no direction but the potential does, the PDF "slides" towards large  $\varphi \rightarrow \infty$ . In the long-time limit, averaged over many periods, the speed of this "sliding" should converge towards a constant value.

### Long-time average of voltage expectation:

We are interested in the long-time average expectation of the voltage  $\overline{\langle V \rangle} = \overline{\langle \dot{\varphi} \rangle}$ . From [subsection 1.4](#), we can interchange the time derivative and expectation:

$$\langle V \rangle = \langle \dot{\varphi} \rangle = \frac{d}{d\tau} \langle \varphi \rangle = \int_{\Omega} \frac{\partial p(\varphi, \tau)}{\partial \tau} \varphi d\varphi$$

The probability follows a continuity equation. We can therefore exchange the time derivative of the probability for the divergence of the probability current ( $\partial p(\varphi, \tau)/\partial \tau = -\partial j(\varphi, \tau)/\partial \varphi$ ):

$$\int_{\Omega} \frac{\partial p(\varphi, \tau)}{\partial \tau} \varphi d\varphi = - \int_{\Omega} \frac{\partial j(\varphi, \tau)}{\partial \varphi} \varphi d\varphi$$

Perform partial integration. The boundary term vanishes, assuming that the PDF is zero at the boundary:

$$- \int_{\Omega} \frac{\partial j(\varphi, \tau)}{\partial \varphi} \varphi d\varphi = -j(\varphi, \tau) \varphi \Big|_{\partial \Omega} + \int_{\Omega} j(\varphi, \tau) d\varphi = \int_{\Omega} j(\varphi, \tau) d\varphi = \langle V \rangle$$

Now take the long-time average:

$$\overline{\langle V \rangle} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \left( \int_{\Omega} j(\varphi, \tau) d\varphi \right) d\tau = \int_{\Omega} \left( \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T j(\varphi, \tau) d\tau \right) d\varphi = \int_{\Omega} \bar{j} d\varphi$$

$$\overline{\langle V \rangle} = \int_{\Omega} \bar{j} d\varphi$$

### Calculate $\bar{j}$ : Take the long-time-average over the Fokker-Planck equation:

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \left( \frac{\partial p(\varphi, \tau)}{\partial \tau} + \frac{\partial j(\varphi, \tau)}{\partial \varphi} \right) d\tau = 0$$

Evaluating the time integrand:

$$\lim_{T \rightarrow \infty} \frac{p(\varphi, T) - p(\varphi, 0)}{T} + \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \frac{\partial j(\varphi, \tau)}{\partial \varphi} d\tau = 0$$

Assume that the diffusion coefficient  $D = b^2/2 > 0$ . Then, the Fokker-Planck equation is a parabolic PDE and its solutions are smooth. One can show via the mean-value theorem

that a continuously differentiable and normalizable PDF  $p(\varphi, \tau)$  over  $(-\infty, \infty)$  must be bounded. In the long-time limit  $T \rightarrow \infty$ , since  $p$  is bounded, the difference quotient vanishes:

$$\lim_{T \rightarrow \infty} \frac{p(\varphi, T) - p(\varphi, 0)}{T} = 0.$$

Since the PDF is smooth, integration and differentiation can be interchanged:

$$\begin{aligned} \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \frac{\partial j}{\partial \varphi} d\tau &= \frac{\partial}{\partial \varphi} \left( \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T j(\varphi, \tau) d\tau \right) = 0 \\ \rightarrow \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T j(\varphi, \tau) d\tau &= \bar{j}(\varphi) = \text{const} = \bar{j} \end{aligned}$$

Here,  $\bar{(\cdot)}$  denotes the time average in the long-time limit. The probability current  $j(\varphi, \tau)$  can be expressed in terms of the PDF  $p(\varphi, \tau)$ :

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T j(\varphi, \tau) d\tau = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \left( (i_0 - \sin(\varphi))p(\varphi, \tau) - D \frac{\partial p(\varphi, \tau)}{\partial \varphi} \right) d\tau$$

Interchange integration and differentiation. Note that  $\varphi$  is not time-dependent in the Fokker-Planck framework:

$$(i_0 - \sin(\varphi)) \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T p(\varphi, \tau) d\tau - D \frac{\partial}{\partial \varphi} \left( \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T p(\varphi, \tau) d\tau \right)$$

Define the long-time average over the PDF as

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T p(\varphi, \tau) d\tau =: \bar{p}(\varphi)$$

With  $\bar{j}(\varphi) = \bar{j} = \text{const}$ , the averaged equation in the long-time limit becomes:

$$\boxed{\bar{j} = (i_0 - \sin(\varphi))\bar{p}(\varphi) - D \frac{d\bar{p}(\varphi)}{d\varphi}} \quad (152)$$

This is a linear first-order ODE. The general solution can be obtained via variations of constants:

$$\begin{aligned} \bar{p}_{\text{hom}}(\varphi) &= C \exp\left(\frac{\cos(\varphi) - 1 + i_0\varphi}{D}\right) \\ \bar{p}_{\text{p}}(\varphi) &= C(\varphi) \exp\left(\frac{\cos(\varphi) - 1 + i_0\varphi}{D}\right) \end{aligned}$$

$$D \frac{d\bar{p}_{\text{p}}(\varphi)}{d\varphi} = (i_0 - \sin(\varphi))\bar{p}_{\text{p}}(\varphi) + D \frac{dC(\varphi)}{d\varphi} \exp\left(\frac{\cos(\varphi) - 1 + i_0\varphi}{D}\right) = (i_0 - \sin(\varphi))\bar{p}_{\text{p}}(\varphi) - \bar{j}$$

The  $(-1)$  was added in the exponent so that the exponential term is  $= 1$  for  $\varphi = 0$ . Since  $\bar{p}_{\text{hom}}(\varphi)$  solves the homogeneous equation, this yields an ODE for  $C(\varphi)$ :

$$\frac{dC(\varphi)}{d\varphi} = -\frac{\bar{j}}{D} \exp\left(-\frac{\cos(\varphi) - 1 + i_0\varphi}{D}\right)$$

Integrating and adding the solutions together (linear ODE), we obtain the general solution

$$\bar{p}(\varphi) = \exp\left(\frac{\cos(\varphi) - 1 + i_0\varphi}{D}\right) \left[ \bar{p}(0) - \frac{\bar{j}}{D} \int_0^\varphi \exp\left(-\frac{\cos(\alpha) - 1 + i_0\alpha}{D}\right) d\alpha \right]$$

Since the driving term (derivative of the potential) is  $2\pi$ -periodic, the long-time average of the PDF should be  $2\pi$ -periodic with  $\bar{p}(\varphi + 2\pi) = \bar{p}(\varphi)$ . This is reasonable, since the PDF is localized but moving with a constant speed (on average), which means that in the long-time limit, the PDF "has been in every periodic spot  $\varphi + 2k\pi$  for exactly the same amount of time".

**Enforce periodic boundary conditions**  $\bar{p}(0) = \bar{p}(2\pi)$ :

$$\bar{p}(2\pi) = \bar{p}(0) = \exp\left(\frac{\cos(2\pi) - 1 + i_0 2\pi}{D}\right) \left[ \bar{p}(0) - \frac{\bar{j}}{D} \int_0^{2\pi} \exp\left(-\frac{\cos(\alpha) - 1 + i_0\alpha}{D}\right) d\alpha \right]$$

Solve for  $\bar{p}(0)$ :

$$\bar{p}(0) = \frac{1}{1 - \exp(-\frac{i_0 2\pi}{D})} \frac{\bar{j}}{D} \int_0^{2\pi} \exp\left(-\frac{\cos(\alpha) - 1 + i_0\alpha}{D}\right) d\alpha$$

Abbreviate the tilted washboard potential  $U(\varphi) := -\cos(\varphi) - i_0\varphi$  and substitute the expression for  $\bar{p}(0)$  into the general solution.

**Enforce normalization:**

$$\int_0^{2\pi} \bar{p}(\varphi) d\varphi = 1 = \int_0^{2\pi} \exp\left(-\frac{U(\varphi) + 1}{D}\right) \left[ \frac{1}{1 - \exp(-\frac{i_0 2\pi}{D})} \frac{\bar{j}}{D} \int_0^{2\pi} \exp\left(\frac{U(\alpha) + 1}{D}\right) d\alpha - \frac{\bar{j}}{D} \int_0^\varphi \exp\left(\frac{U(\alpha) + 1}{D}\right) d\alpha \right] d\varphi$$

Factor out  $\exp(-1/D)$  and  $\exp(1/D)$ , respectively. These terms cancel out and we are left with

$$1 = \frac{\bar{j}}{D} \int_0^{2\pi} \exp\left(-\frac{U(\varphi)}{D}\right) \left[ \frac{1}{1 - \exp(-\frac{i_0 2\pi}{D})} \int_0^{2\pi} \exp\left(\frac{U(\alpha)}{D}\right) d\alpha - \int_0^\varphi \exp\left(\frac{U(\alpha)}{D}\right) d\alpha \right] d\varphi$$

Bring  $\bar{j}/D$  to the LHS and multiply both sides by  $1 - \exp(-i_0 2\pi/D)$ :

$$\begin{aligned} & \frac{D}{\bar{j}} \left( 1 - \exp\left(-\frac{i_0 2\pi}{D}\right) \right) \\ &= \int_0^{2\pi} \exp\left(-\frac{U(\varphi)}{D}\right) \left[ \int_0^{2\pi} \exp\left(\frac{U(\alpha)}{D}\right) d\alpha - \int_0^\varphi \exp\left(\frac{U(\alpha)}{D}\right) d\alpha + \int_0^\varphi \exp\left(\frac{U(\alpha) - i_0 2\pi}{D}\right) d\alpha \right] d\varphi \end{aligned}$$

Pull the first two integrals over  $\alpha$  together. Perform a coordinate transform for the third integral ( $U(\alpha) - i_0 2\pi = -\cos(\alpha) - i_0(\alpha - 2\pi)$ ) with  $\alpha \rightarrow \alpha + 2\pi$ : The exponent becomes  $(-\cos(\alpha) - i_0\alpha = U(\alpha))$  and the integral limits become  $\varphi, \varphi + 2\pi$

$$\frac{D}{\bar{j}} \left( 1 - \exp\left(-\frac{i_0 2\pi}{D}\right) \right) = \int_0^{2\pi} \exp\left(-\frac{U(\varphi)}{D}\right) \left[ \int_\varphi^{2\pi} \exp\left(\frac{U(\alpha)}{D}\right) d\alpha + \int_{2\pi}^{\varphi+2\pi} \exp\left(\frac{U(\alpha)}{D}\right) d\alpha \right] d\varphi$$



Pull the remaining two integrals over  $\alpha$  together:

$$\frac{D}{j} \left( 1 - \exp\left(-\frac{i_0 2\pi}{D}\right) \right) = \int_0^{2\pi} \int_{\varphi}^{2\pi+\varphi} \exp\left(-\frac{U(\varphi)}{D}\right) \exp\left(\frac{U(\alpha)}{D}\right) d\alpha d\varphi$$

Perform a coordinate transform  $\alpha \rightarrow \alpha + \varphi$ . The new integral limits become  $0, 2\pi$ :

$$\frac{D}{j} \left( 1 - \exp\left(-\frac{i_0 2\pi}{D}\right) \right) = \int_0^{2\pi} \int_0^{2\pi} \exp\left(-\frac{U(\varphi)}{D}\right) \exp\left(\frac{U(\alpha + \varphi)}{D}\right) d\alpha d\varphi$$

Substitute in the expression for the tilted washboard potential  $U$ :

$$= \int_0^{2\pi} \int_0^{2\pi} \exp\left(\frac{\cos(\varphi) + i_0 \varphi}{D}\right) \exp\left(\frac{-\cos(\varphi + \alpha) - i_0(\varphi + \alpha)}{D}\right) d\alpha d\varphi$$

Simplify:

$$= \int_0^{2\pi} \int_0^{2\pi} \exp\left(\frac{\cos(\varphi) - \cos(\varphi + \alpha) - i_0 \alpha}{D}\right) d\alpha d\varphi =: \Pi$$

Try to simplify the double integral on the RHS further: First, reformulate the exponent by using the identity

$$\begin{aligned} \cos(A) - \cos(B) &= -2 \sin\left(\frac{A+B}{2}\right) \sin\left(\frac{A-B}{2}\right) \\ \cos(\varphi) - \cos(\varphi + \alpha) &= -2 \sin\left(\frac{2\varphi + \alpha}{2}\right) \sin\left(-\frac{\alpha}{2}\right) = 2 \sin\left(\varphi + \frac{\alpha}{2}\right) \sin\left(\frac{\alpha}{2}\right) \end{aligned}$$

The integrand can then be expressed as:

$$\exp\left(\frac{\cos(\varphi) - \cos(\varphi + \alpha) - i_0 \alpha}{D}\right) = \exp\left(-\frac{i_0 \alpha}{D}\right) \exp\left(\frac{2 \sin\left(\varphi + \frac{\alpha}{2}\right) \sin\left(\frac{\alpha}{2}\right)}{D}\right)$$

The second term resembles the generating function of the Bessel functions of first kind (Jacobi-Anger expansion):

$$\begin{aligned} e^{iz \cos(\phi)} &= \sum_{n=-\infty}^{\infty} i^n J_n(x) e^{in\phi} = \sum_{n=-\infty}^{\infty} J_n(x) e^{in(\phi+\pi/2)} \\ &\rightarrow \sum_{n=-\infty}^{\infty} J_n(x) e^{in\phi} = e^{iz \cos(\phi-\pi/2)} = e^{iz \sin(\phi)} \end{aligned}$$

Where the Bessel function  $J_m(z)$  is defined as the series

$$J_n(z) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m! \Gamma(m+n+1)} \left(\frac{z}{2}\right)^{2m+n}$$

For imaginary  $z = iy$ ,  $J_n(iy) = I_n(y)$  where  $I_n(y)$  are the modified Bessel functions

$$I_n(y) = \sum_{m=0}^{\infty} \frac{1}{m! \Gamma(m+n+1)} \left(\frac{y}{2}\right)^{2m+n}$$

Rewrite the exponent:

$$\exp\left(\frac{2\sin\left(\varphi + \frac{\alpha}{2}\right)\sin\left(\frac{\alpha}{2}\right)}{D}\right) = \exp\left(i\left(-\frac{2i\sin\left(\frac{\alpha}{2}\right)}{D}\right)\sin\left(\varphi + \frac{\alpha}{2}\right)\right)$$

Use the Jacobi-Anger expansion (generating function of the Bessel functions of first kind):

$$\exp\left(i\left(-\frac{2i\sin\left(\frac{\alpha}{2}\right)}{D}\right)\sin\left(\varphi + \frac{\alpha}{2}\right)\right) = \sum_{n=-\infty}^{\infty} J_n\left(-\frac{2i\sin\left(\frac{\alpha}{2}\right)}{D}\right) \exp\left(in\left(\varphi + \frac{\alpha}{2}\right)\right)$$

Using  $J_n(iy) = I_n(y)$  and  $I_n(-y) = I_n(y)$  and integrating over  $\varphi$ :

$$\begin{aligned} \Pi &= \int_0^{2\pi} \int_0^{2\pi} \exp\left(\frac{\cos(\varphi) - \cos(\varphi + \alpha) - i_0\alpha}{D}\right) d\varphi d\alpha \\ &= \int_0^{2\pi} \left[ \int_0^{2\pi} \left( \exp\left(-\frac{i_0\alpha}{D}\right) \sum_{n=-\infty}^{\infty} I_n\left(\frac{2\sin\left(\frac{\alpha}{2}\right)}{D}\right) \exp\left(in\left(\varphi + \frac{\alpha}{2}\right)\right) \right) d\varphi \right] d\alpha \\ &= \sum_{n=-\infty}^{\infty} \int_0^{2\pi} \left( \exp\left(-\frac{i_0\alpha}{D}\right) I_n\left(\frac{2\sin\left(\frac{\alpha}{2}\right)}{D}\right) \exp\left(in\frac{\alpha}{2}\right) \right) d\alpha \int_0^{2\pi} \exp(in\varphi) d\varphi \end{aligned}$$

The integral over  $\varphi$  is zero for all elements of the sum except  $n = 0$  where it amounts to  $2\pi$  (because of the periodicity of  $\exp(in\varphi)$ ):

$$\Pi = 2\pi \int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) I_0\left(\frac{2\sin\left(\frac{\alpha}{2}\right)}{D}\right) d\alpha$$

This is a somewhat nice expression for the RHS. Rearrange the equation with respect to  $\bar{j}$ :

$$\begin{aligned} \frac{D}{\bar{j}} \left(1 - \exp\left(-\frac{i_0 2\pi}{D}\right)\right) &= 2\pi \int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) I_0\left(\frac{2\sin\left(\frac{\alpha}{2}\right)}{D}\right) d\alpha \\ \rightarrow \bar{j} &= \frac{D \left(1 - \exp\left(-\frac{i_0 2\pi}{D}\right)\right)}{2\pi \int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) I_0\left(\frac{2\sin\left(\frac{\alpha}{2}\right)}{D}\right) d\alpha} \end{aligned}$$

From [Equation 152](#), relate the long-time average of the voltage  $\overline{\langle V \rangle}$  to the long-time average of the probability current  $\bar{j}$ :

$$\overline{\langle V \rangle} = \int_0^{2\pi} \bar{j} d\varphi = 2\pi \bar{j}$$

Substitute  $\overline{\langle V \rangle}$  for  $\bar{j}$ :

$$\boxed{\overline{\langle V \rangle} = \frac{D \left(1 - \exp\left(-\frac{i_0 2\pi}{D}\right)\right)}{\int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) I_0\left(\frac{2\sin\left(\frac{\alpha}{2}\right)}{D}\right) d\alpha}} \quad (153)$$

Trying to further simplify the integral in the numerator: Express  $I_0$  via its series expansion:

$$\Pi = \int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) \sum_{m=0}^{\infty} \frac{1}{(m!)^2} \left(\frac{\sin(\frac{\alpha}{2})}{D}\right)^{2m} d\alpha$$

Pull the sum in front of the integral:

$$= \sum_{m=0}^{\infty} \frac{1}{(m!)^2 D^{2m}} \int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) \sin^{2m}\left(\frac{\alpha}{2}\right) d\alpha$$

Perform the substitution  $x = \alpha/2$ :

$$= 2 \sum_{m=0}^{\infty} \frac{1}{(m!)^2 D^{2m}} \int_0^{\pi} \exp\left(-\frac{2i_0x}{D}\right) \sin^{2m}(x) dx$$

This integral has known solutions (can be obtained by partially integrating  $2m$  times (yikes):

$$\begin{aligned} &= 2 \sum_{m=0}^{\infty} \frac{1}{(m!)^2 D^{2m}} \frac{(2m)! \left(1 - \exp\left(-\frac{2\pi i_0}{D}\right)\right)}{\frac{2i_0}{D} \left(\left(\frac{2i_0}{D}\right)^2 + 2^2\right) \left(\left(\frac{2i_0}{D}\right)^2 + 4^2\right) \dots \left(\left(\frac{2i_0}{D}\right)^2 + (2m)^2\right)} \\ &= 2 \left(1 - \exp\left(-\frac{2\pi i_0}{D}\right)\right) \sum_{m=0}^{\infty} \frac{1}{(m!)^2 D^{2m}} \frac{(2m)!}{\frac{2i_0}{D} \prod_{n=0}^m \left(\left(\frac{2i_0}{D}\right)^2 + (2n)^2\right)} \\ &= 2 \left(1 - \exp\left(-\frac{2\pi i_0}{D}\right)\right) \sum_{m=0}^{\infty} \frac{1}{(m!)^2 D^{2m}} \frac{(2m)!}{\frac{2i_0}{D} \left(\frac{2i_0}{D}\right)^{2m} \prod_{n=0}^m \left(1 + \left(n \frac{D}{i_0}\right)^2\right)} \\ &= \frac{D}{i_0} \left(1 - \exp\left(-\frac{2\pi i_0}{D}\right)\right) \sum_{m=0}^{\infty} \frac{(2m)!}{(m!)^2 (2i_0)^{2m}} \frac{1}{\prod_{n=0}^m \left(1 + \left(n \frac{D}{i_0}\right)^2\right)} \\ &= \frac{D}{i_0} \left(1 - \exp\left(-\frac{2\pi i_0}{D}\right)\right) \sum_{m=0}^{\infty} \binom{2m}{m} \left(\frac{1}{4i_0^2}\right)^m \frac{1}{\prod_{n=0}^m \left(1 + \left(n \frac{D}{i_0}\right)^2\right)} \quad \text{where } \frac{(2m)!}{(m!)^2} = \binom{2m}{m} \end{aligned}$$

Substitute this expression into [Equation 153](#):

$$\overline{\langle V \rangle} = \frac{i_0}{\sum_{m=0}^{\infty} \binom{2m}{m} \left(\frac{1}{4i_0^2}\right)^m \frac{1}{\prod_{n=0}^m \left(1 + \left(n \frac{D}{i_0}\right)^2\right)}} \quad (154)$$

**For no noise** ( $D \rightarrow 0$ ), this expression simplifies to

$$\begin{aligned}\overline{\langle V \rangle} &= \frac{i_0}{\sum_{m=0}^{\infty} \binom{2m}{m} \left(\frac{1}{4i_0^2}\right)^m}, \left(\sum_{m=0}^{\infty} \binom{2m}{m} x^m = \frac{1}{\sqrt{1-4x}}, x < \frac{1}{4}\right) \\ &= i_0 \sqrt{1 - 4\frac{1}{4i_0^2}}, \quad \frac{1}{4i_0^2} < \frac{1}{4} \\ &= \sqrt{i_0^2 - 1}, \quad i_0 > 1\end{aligned}$$

where  $1/\sqrt{1-4x}$  is the generating function of the central binomial coefficient  $\binom{2m}{m}$  (see Wikipedia). For  $i_0 \leq 1$ , the series diverges, which can be shown via the ratio test (Quotientenkriterium)  $\rightarrow \overline{\langle V \rangle} = 0$

**For finite noise**  $D \gg 2$ , we can approximate the Bessel function: Perform partial integration on the integral in the numerator in [Equation 153](#):

$$\begin{aligned}\text{II} = \int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) I_0\left(\frac{2\sin(\frac{\alpha}{2})}{D}\right) d\alpha &= -\frac{D}{i_0} \exp\left(-\frac{i_0\alpha}{D}\right) I_0\left(\frac{2\sin(\frac{\alpha}{2})}{D}\right) \Bigg|_0^{2\pi} \\ &\quad + \frac{D}{i_0} \int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) \frac{d}{d\alpha} \left(I_0\left(\frac{2\sin(\frac{\alpha}{2})}{D}\right)\right) d\alpha\end{aligned}$$

The derivative of the Bessel function of first kind is

$$\frac{dI_0(x)}{dx} = I_1(x)$$

With  $I_0(0) = 1$ :

$$\text{II} = \frac{D}{i_0} \left(1 - \exp\left(-\frac{i_0 2\pi}{D}\right)\right) + \frac{D}{i_0} \int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) \frac{\cos(\frac{\alpha}{2})}{D} I_1\left(\frac{2\sin(\frac{\alpha}{2})}{D}\right) d\alpha$$

For  $x < 1$ ,  $I_1(x)$  can be approximated as

$$I_1(x) = \frac{x}{2} + \frac{x^3}{16} + \frac{x^5}{384} + \dots \approx \frac{x}{2}$$

This approximation yields an error of around 3% for  $x \lesssim 0.5$ .

Substitute and simplify:

$$\begin{aligned}\text{II} &= \frac{D}{i_0} \left(1 - \exp\left(-\frac{i_0 2\pi}{D}\right)\right) + \frac{D}{i_0 D^2} \int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) \cos\left(\frac{\alpha}{2}\right) \sin\left(\frac{\alpha}{2}\right) d\alpha \\ &= \frac{D}{i_0} \left(1 - \exp\left(-\frac{i_0 2\pi}{D}\right) - \frac{1}{D} \left[ D \exp\left(-\frac{i_0\alpha}{D}\right) \frac{i_0 \sin(\alpha) + D \cos(\alpha)}{2(i_0^2 + D^2)} \right] \Bigg|_0^{2\pi} \right) \\ &= \frac{D}{i_0} \left(1 - \exp\left(-\frac{i_0 2\pi}{D}\right) - \frac{D}{2(i_0^2 + D^2)} \left(\exp\left(-\frac{i_0 2\pi}{D}\right) - 1\right)\right)\end{aligned}$$

Substitute the results for the approximate integral into [Equation 153](#):

$$\overline{\langle V \rangle} \approx \frac{D \left( 1 - \exp \left( -\frac{i_0 2\pi}{D} \right) \right)}{\frac{D}{i_0} \left( 1 - \exp \left( -\frac{i_0 2\pi}{D} \right) + \frac{D}{2(i_0^2 + D^2)} \left( 1 - \exp \left( -\frac{i_0 2\pi}{D} \right) \right) \right)} = \frac{i_0}{1 + \frac{D}{2(i_0^2 + D^2)}}$$

**For infinite noise** ( $D \rightarrow \infty$ ), we can directly see that  $\overline{\langle V \rangle} \rightarrow i_0$ . This can also be obtained from the series expression: the product in the numerator is  $\infty$  except for  $m = 0$ , which leads to all elements of the sum being 0 except for the first element. The first element of the series ( $m = 0$ ) is simply  $= 1$ , leading to:

$$\overline{\langle V \rangle} = \frac{i_0}{\sum_{m=0}^{\infty} \binom{2m}{m} \left( \frac{1}{4i_0^2} \right)^m \frac{1}{\prod_{n=0}^m \left( 1 + \left( n \frac{D}{i_0} \right)^2 \right)}} = \frac{i_0}{\binom{0}{0} \left( \frac{1}{4i_0^2} \right)^0} = i_0$$

### 8.3 Numerical Solution

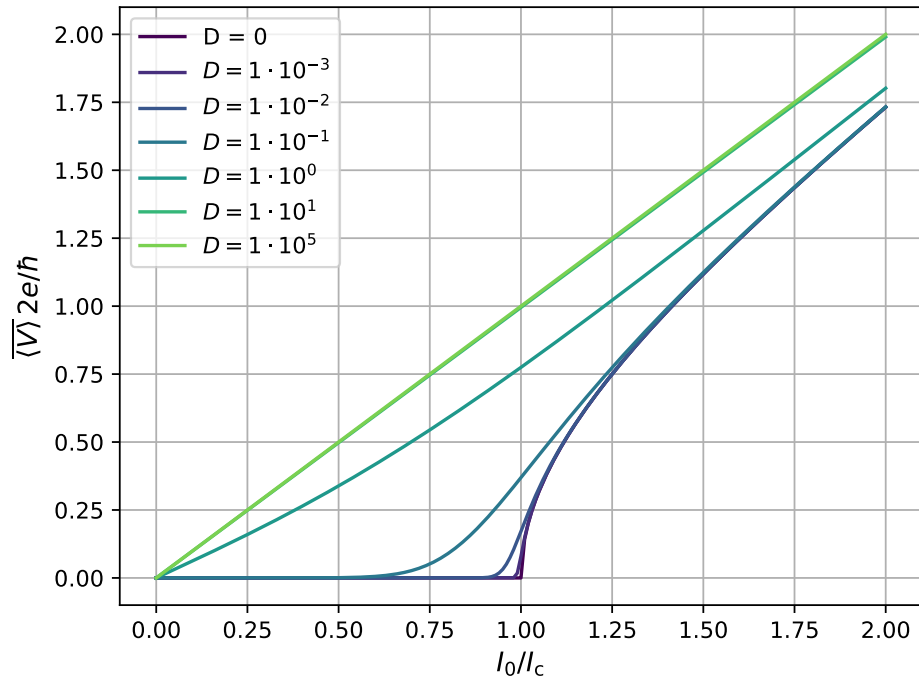


Figure 13: Analytically calculated I-V curve for different diffusion coefficients  $D = \frac{k_B T}{E_J}$

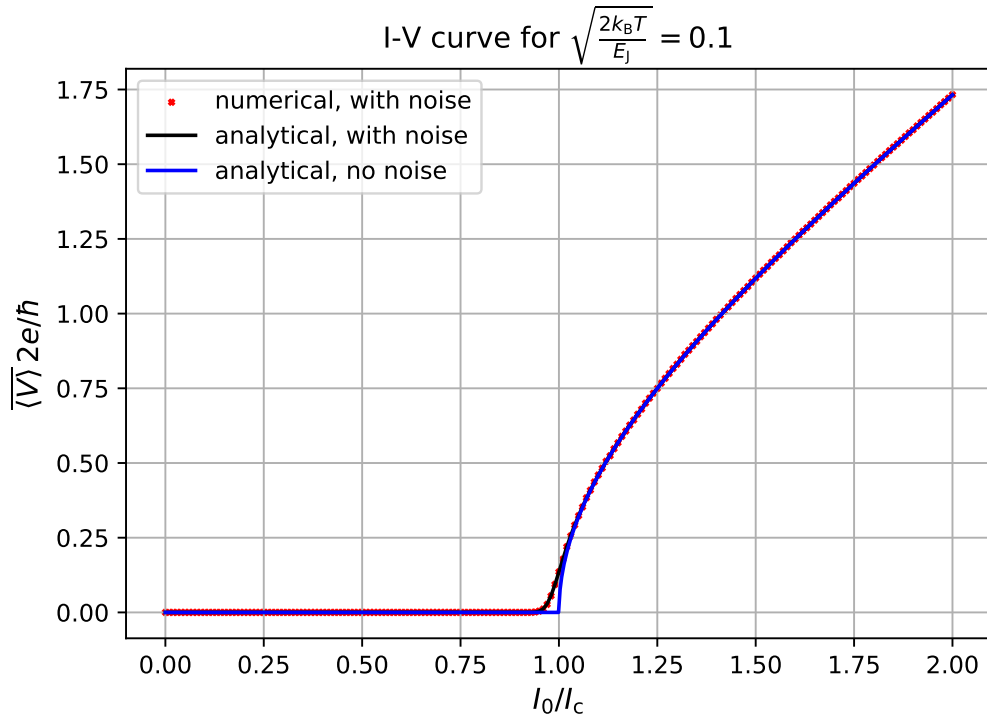


Figure 14: I-V curve for  $\sqrt{2D} = 0.1$ .  $T = 10^5$ ,  $N_T = 10^6$ . Averaged over  $10^3$  permutations

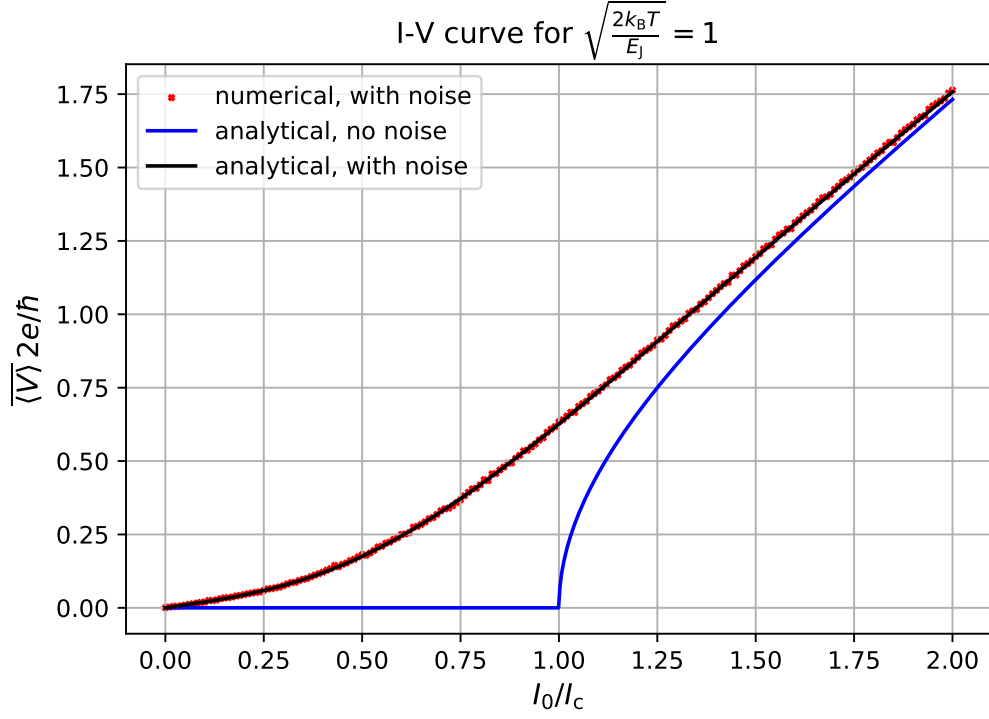


Figure 15: I-V curve for  $\sqrt{2D} = 1$ .  $T = 2 \cdot 10^5$ ,  $N_T = 10^6$ . Averaged over  $10^3$  permutations

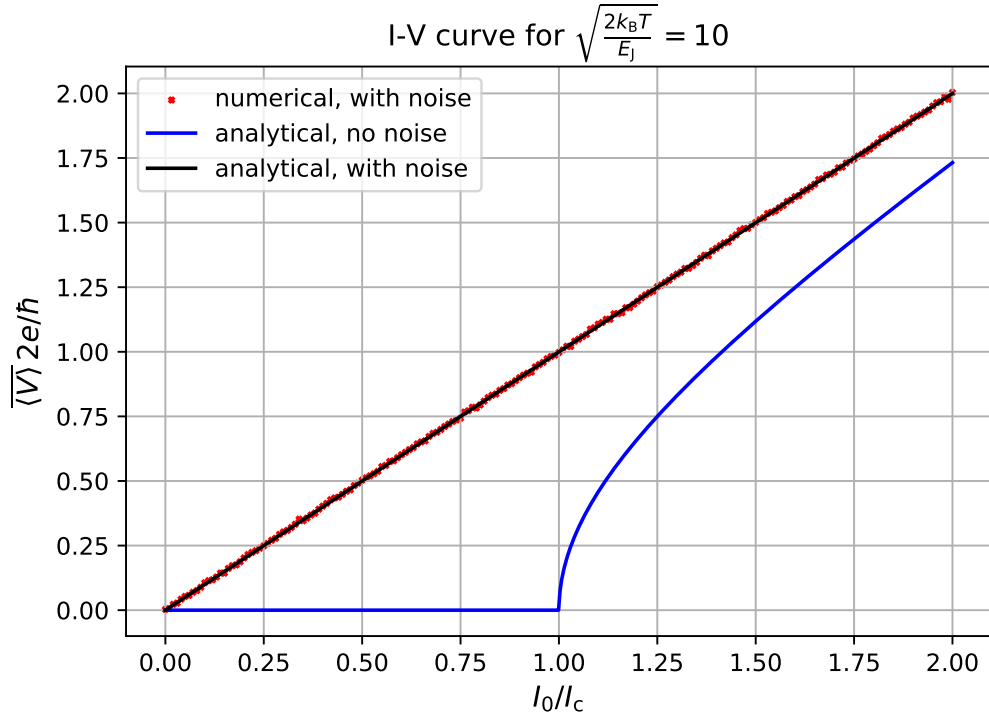


Figure 16: I-V curve for  $\sqrt{2D} = 10$ .  $T = 10^7$ ,  $N_T = 10^6$ . Averaged over  $10^3$  permutations

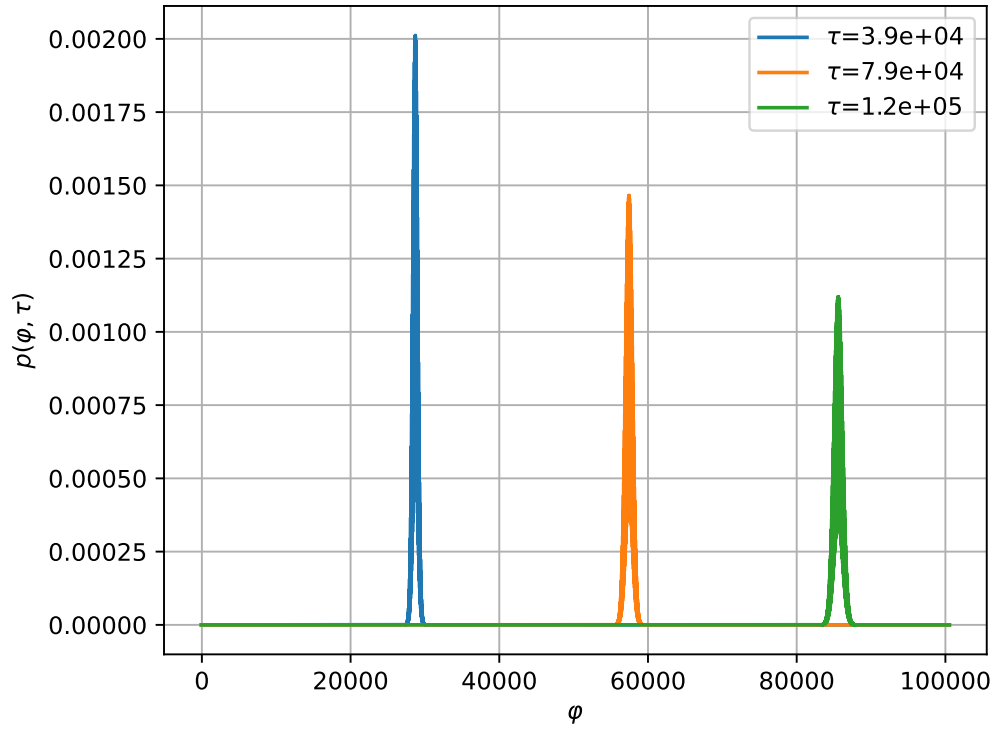


Figure 17: PDF for  $i_0 = D = 1$

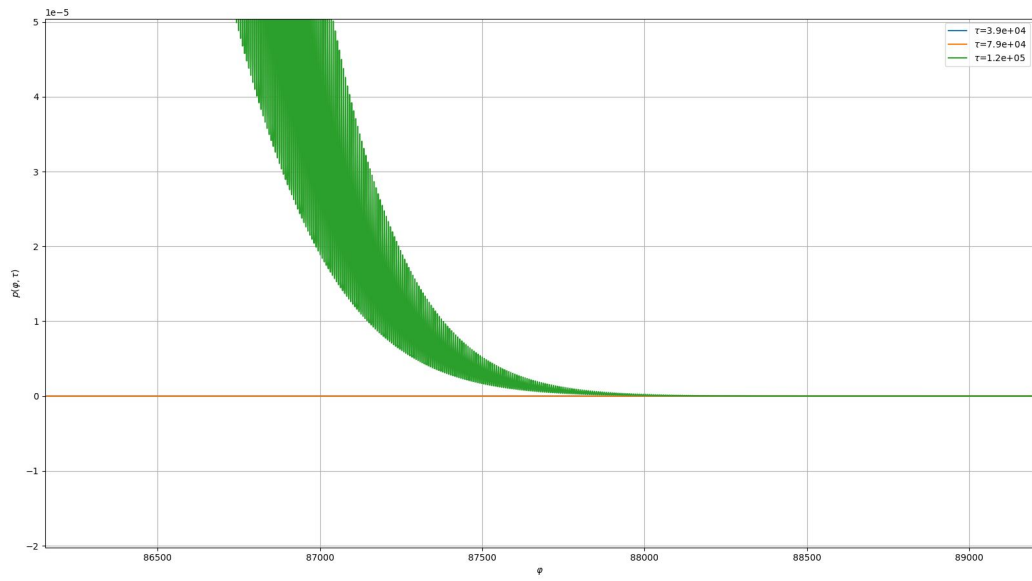


Figure 18: PDF zoomed in for  $i_0 = D = 1$



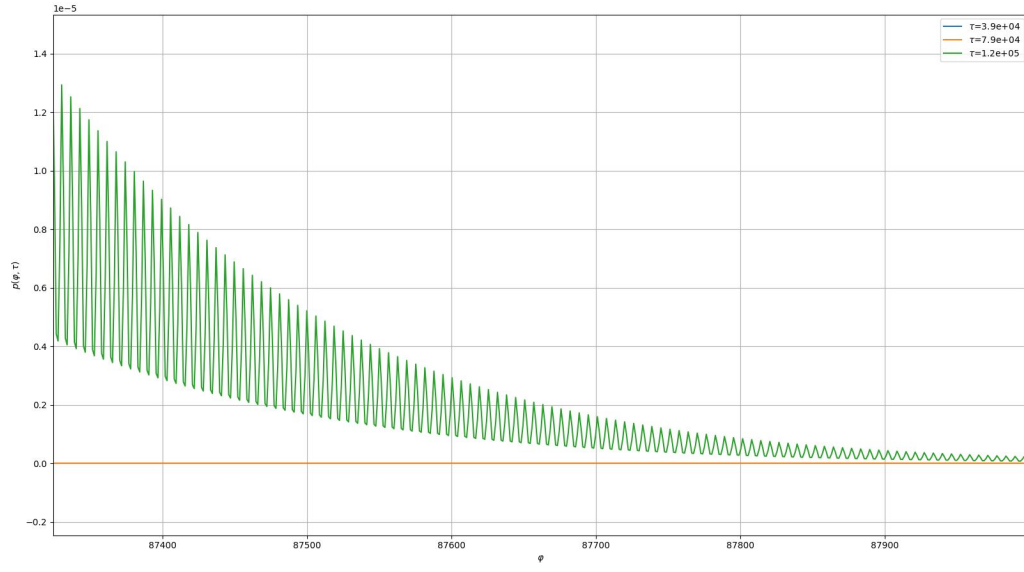


Figure 19: PDF zoomed in for  $i_0 = D = 1$

## 8.4 Approach via First Passage Time and the Renewal Theory CLT

### 8.4.1 First Passage Time

Define the first passage time  $\tau_\beta$  as the time at which the system first reaches the state  $\beta$ :

$$\tau_\beta = \inf[t \geq 0 | \mathbf{x}_t = \beta]$$

Define the mean first passage time (MFPT)  $T_1(\mathbf{x} \rightarrow \beta)$  time as the expected time it takes until the system first reaches the state  $\beta$ , given that it is in state  $\mathbf{x}_0 = \mathbf{x}$  at time 0:

$$T_1(\mathbf{x} \rightarrow \beta) = \mathbb{E}[\tau_\beta | \mathbf{x}_0 = x]$$

The MFPT is then governed by the Kolmogorov backward equation (see [subsection 1.10](#)) with  $\partial T_1(\mathbf{x} \rightarrow \beta) / \partial \tau = 1$  (since time passes linearly):

$$\mathbf{a} \cdot \nabla T_1(\mathbf{x} \rightarrow \beta) + \frac{1}{2} \text{Tr}(\mathbf{B}\mathbf{B}_1^T \nabla^2 T(\mathbf{x} \rightarrow \beta)) = -1 \quad (155)$$

One boundary condition is  $T_1(\mathbf{x} = \beta \rightarrow \beta) = 0$  (it takes 0 time to arrive at  $\beta$  if you're already there). The second boundary condition depends on the drift. One boundary condition that must always be fulfilled is that  $T_1(\mathbf{x} \rightarrow \beta) \geq 0$

Higher moments of the first passage time  $T_n(\mathbf{x} \rightarrow \beta) := \mathbb{E}[\tau_\beta^n | \mathbf{x}_0 = x]$  can also be computed via the Kolmogorov backward equation: The time derivative

$$\begin{aligned} \frac{\partial T_1(\mathbf{x} \rightarrow \beta)}{\partial \tau} &= 1 \\ \frac{\partial T_n(\mathbf{x} \rightarrow \beta)}{\partial \tau} &= n T_{n-1}(\mathbf{x} \rightarrow \beta) \end{aligned}$$

for example for the second moment  $\mathbb{E}[\tau^2 | \mathbf{x}_0 = x]$ :

$$\frac{\partial T_2(\mathbf{x} \rightarrow \beta)}{\partial \tau} = 2 T_1(\mathbf{x} \rightarrow \beta)$$

Which would need to be computed via

$$\mathbf{a} \cdot \nabla T_2(\mathbf{x} \rightarrow \beta) + \frac{1}{2} \text{Tr}(\mathbf{B}\mathbf{B}_2^T \nabla^2 T(\mathbf{x} \rightarrow \beta)) = -2 T_1(\mathbf{x} \rightarrow \beta)$$

### 8.4.2 Mean of the First Passage Time

The MFPT is governed by the second-order linear ODE (see [subsection 1.10](#) and [subsection 8.4.1](#))

$$(i_0 - \sin(\varphi)) \frac{dT_1(\varphi \rightarrow \beta)}{d\varphi} + D \frac{d^2 T_1(\varphi \rightarrow \beta)}{d\varphi^2} = -1$$

One boundary condition is  $T_1(\varphi = \beta \rightarrow \beta) = 0$  (see [Equation 155](#)). The second boundary condition is  $T_1(\varphi \rightarrow \beta) \geq 0$  for  $\varphi \leq \beta$

Substitute  $z = T_1'$ . This yields the ODE

$$\frac{dz}{d\varphi} + \frac{i_0 - \sin(\varphi)}{D} z = -\frac{1}{D}$$

The general solution is

$$z(\varphi) = \exp\left(-\frac{i_0\varphi + \cos(\varphi)}{D}\right) \left(C_1 - \frac{1}{D} \int_{\beta}^{\varphi} \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi''\right)$$

Integrating once yields the solution for  $T_1(\varphi \rightarrow \beta)$ :

$$\begin{aligned} T_1(\varphi \rightarrow \beta) &= \int_0^{\varphi} z(\varphi') d\varphi' \\ &= \int_{\beta}^{\varphi} \left[ \exp\left(-\frac{i_0\varphi' + \cos(\varphi')}{D}\right) \left(C_1 - \frac{1}{D} \int_{\beta}^{\varphi'} \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi''\right) \right] d\varphi' + C_2 \end{aligned}$$

From the boundary condition  $T_1((\varphi = \beta) \rightarrow \beta) = 0$ , we obtain that  $C_2 = 0$ .

From the condition that  $T_1(\varphi \rightarrow \beta) \geq 0$  for  $\varphi \leq \beta$ , we can derive a constraint for  $C_1$ :

$$\int_{\beta}^{\varphi} \left[ \exp\left(-\frac{i_0\varphi' + \cos(\varphi')}{D}\right) \left(C_1 - \frac{1}{D} \int_{\beta}^{\varphi'} \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi''\right) \right] d\varphi' \geq 0 \quad \text{for all } \varphi \leq \beta$$

Flipping the integral boundaries on the outer integral and flipping signs on the inner integrand preserves the sign of the entire term:

$$\int_{\varphi}^{\beta} \left[ \exp\left(-\frac{i_0\varphi' + \cos(\varphi')}{D}\right) \left(-\frac{1}{D} \int_{\varphi'}^{\beta} \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' - C_1\right) \right] d\varphi' \geq 0 \quad \text{for all } \varphi \leq \beta$$

The first exponential term is always  $\geq 0$ . This puts the constraint on the inner term:

$$-\frac{1}{D} \int_{\varphi'}^{\beta} \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' \geq C_1 \quad \text{for all } \varphi' \leq \beta$$

Since the integrand is always  $\geq 0$ , the integral is ever-decreasing for decreasing  $\varphi'$ . This means that the only  $C_1$  that fulfills this constraint is

$$C_1 = -\frac{1}{D} \int_{-\infty}^{\beta} \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi''$$

Substituting back and flipping the integration boundaries in the outer integral:

$$\begin{aligned}
T_1(\varphi \rightarrow \beta) &= \int_{\varphi}^{\beta} \left[ \exp\left(-\frac{i_0\varphi' + \cos(\varphi')}{D}\right) \right. \\
&\quad \left. \left( \frac{1}{D} \int_{-\infty}^{\beta} \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' + \frac{1}{D} \int_{\beta}^{\varphi'} \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' \right) \right] d\varphi' \\
&= \frac{1}{D} \int_{\varphi}^{\beta} \left[ \exp\left(-\frac{i_0\varphi' + \cos(\varphi')}{D}\right) \int_{-\infty}^{\varphi'} \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' \right] d\varphi'
\end{aligned}$$

Expand the inner integral as a series:

$$\begin{aligned}
\int_{-\infty}^{\varphi'} \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' &= \sum_{k=0}^{\infty} \int_{\varphi' - 2(k+1)\pi}^{\varphi' - 2k\pi} \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' \\
&= \sum_{k=0}^{\infty} \int_{\varphi' - 2\pi}^{\varphi'} \exp\left(\frac{i_0(\varphi'' - 2k\pi) + \cos(\varphi'' - 2k\pi)}{D}\right) d\varphi'' \\
&= \int_{\varphi' - 2\pi}^{\varphi'} \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' \sum_{k=0}^{\infty} \left(e^{-\frac{2\pi i_0}{D}}\right)^k \\
&= \int_{\varphi' - 2\pi}^{\varphi'} \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' \frac{1}{1 - \exp\left(-\frac{2\pi i_0}{D}\right)}
\end{aligned}$$

Shift the integral bounds in the inner integral to 0 and  $2\pi$  by substituting  $\alpha = -\varphi'' + \varphi'$ . The inner integral becomes

$$\begin{aligned}
\int_{\varphi' - 2\pi}^{\varphi'} \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' &= - \int_{2\pi}^0 \exp\left(\frac{i_0(-\alpha + \varphi') + \cos(-\alpha + \varphi')}{D}\right) d\alpha \\
&= \int_0^{2\pi} \exp\left(\frac{i_0(\varphi' - \alpha) + \cos(\varphi' - \alpha)}{D}\right) d\alpha
\end{aligned}$$

Substitute back:

$$\begin{aligned}
T_1(\varphi \rightarrow \beta) &= \frac{1}{D(1 - \exp(-\frac{2\pi i_0}{D}))} \int_{\varphi}^{\beta} \left[ \exp\left(-\frac{i_0\varphi' + \cos(\varphi')}{D}\right) \int_0^{2\pi} \exp\left(\frac{i_0(\varphi' - \alpha) + \cos(\varphi' - \alpha)}{D}\right) d\alpha \right] d\varphi' \\
&= \frac{1}{D(1 - \exp(-\frac{2\pi i_0}{D}))} \int_{\varphi}^{\beta} \left[ \int_0^{2\pi} \exp\left(\frac{-i_0\alpha + \cos(\varphi' - \alpha) - \cos(\varphi')}{D}\right) d\alpha \right] d\varphi'
\end{aligned}$$

Try to simplify the double integral further: First, reformulate the exponent by using the identity

$$\begin{aligned}
\cos(A) - \cos(B) &= -2 \sin\left(\frac{A+B}{2}\right) \sin\left(\frac{A-B}{2}\right) \\
\cos(\varphi' - \alpha) - \cos(\varphi') &= -2 \sin\left(\frac{2\varphi' - \alpha}{2}\right) \sin\left(-\frac{\alpha}{2}\right) = 2 \sin\left(\varphi' - \frac{\alpha}{2}\right) \sin\left(\frac{\alpha}{2}\right)
\end{aligned}$$

The integrand can then be expressed as:

$$\exp\left(\frac{-i_0\alpha + \cos(\varphi' - \alpha) - \cos(\varphi')}{D}\right) = \exp\left(-\frac{i_0\alpha}{D}\right) \exp\left(\frac{2\sin(\varphi' - \frac{\alpha}{2})\sin(\frac{\alpha}{2})}{D}\right)$$

Thus

$$T_1(\varphi \rightarrow \beta) = \frac{1}{D(1 - \exp(-\frac{2\pi i_0}{D}))} \int_{\varphi}^{\beta} \left[ \int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) \exp\left(\frac{2\sin(\varphi' - \frac{\alpha}{2})\sin(\frac{\alpha}{2})}{D}\right) d\alpha \right] d\varphi'$$

One can show that

$$\begin{aligned} T_1(\varphi \rightarrow \varphi + 2\pi n) &= \frac{1}{D(1 - \exp(-\frac{2\pi i_0}{D}))} \int_{\varphi}^{\varphi+2\pi n} \left[ \int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) \exp\left(\frac{2\sin(\varphi' - \frac{\alpha}{2})\sin(\frac{\alpha}{2})}{D}\right) d\alpha \right] d\varphi' \\ &= \frac{1}{D(1 - \exp(-\frac{2\pi i_0}{D}))} \sum_{k=0}^{n-1} \int_{\varphi+2\pi k}^{\varphi+2\pi(k+1)} \left[ \int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) \exp\left(\frac{2\sin(\varphi' - \frac{\alpha}{2})\sin(\frac{\alpha}{2})}{D}\right) d\alpha \right] d\varphi' \\ &= \frac{n}{D(1 - \exp(-\frac{2\pi i_0}{D}))} \int_{\varphi}^{\varphi+2\pi} \left[ \int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) \exp\left(\frac{2\sin(\varphi' - \frac{\alpha}{2})\sin(\frac{\alpha}{2})}{D}\right) d\alpha \right] d\varphi' \end{aligned}$$

For  $\varphi = 0$  and  $\beta = 2\pi$ , in analogy to [subsection 8.2](#), the integrand can be expressed in terms of the generating function of the Bessel functions of first kind  $J_n$ : Using  $J_n(iy) = I_n(y)$  and  $I_n(-y) = I_n(y)$  and integrating over  $\varphi'$ :

$$\begin{aligned} &\int_0^{2\pi} \left[ \int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) \exp\left(\frac{2\sin(\varphi' - \frac{\alpha}{2})\sin(\frac{\alpha}{2})}{D}\right) d\alpha \right] d\varphi' \\ &= \int_0^{2\pi} \left[ \int_0^{2\pi} \left( \exp\left(-\frac{i_0\alpha}{D}\right) \sum_{n=-\infty}^{\infty} I_n\left(\frac{2\sin(\frac{\alpha}{2})}{D}\right) \exp\left(in\left(\varphi' - \frac{\alpha}{2}\right)\right) \right) d\varphi' \right] d\alpha \\ &= \sum_{n=-\infty}^{\infty} \int_0^{2\pi} \left( \exp\left(-\frac{i_0\alpha}{D}\right) I_n\left(\frac{2\sin(\frac{\alpha}{2})}{D}\right) \exp\left(-in\frac{\alpha}{2}\right) \right) d\alpha \int_0^{2\pi} \exp(in\varphi') d\varphi' \\ &= 2\pi \int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) I_0\left(\frac{2\sin(\frac{\alpha}{2})}{D}\right) d\alpha \end{aligned}$$

The integral over  $\varphi'$  is zero for all elements of the sum except  $n = 0$  where it amounts to  $2\pi$  (because of the periodicity of  $\exp(in\varphi')$ ). Note that the sign is flipped for the rotating terms in the exponent compared to [subsection 8.2](#).

Substituting back yields the expression:

$$T_1(0 \rightarrow 2\pi) = \frac{2\pi}{D(1 - \exp(-\frac{2\pi i_0}{D}))} \int_0^{2\pi} \exp\left(-\frac{i_0\alpha}{D}\right) I_0\left(\frac{2\sin(\frac{\alpha}{2})}{D}\right) d\alpha \quad (156)$$

And for arbitrary  $\varphi$ :

$$T_1(\varphi \rightarrow \varphi + d\varphi) = \frac{1}{D(1 - \exp(-\frac{2\pi i_0}{D}))} \left[ \int_0^{2\pi} \exp\left(\frac{-i_0\alpha + \cos(\varphi - \alpha) - \cos(\varphi)}{D}\right) d\alpha \right] d\varphi$$

### 8.4.3 Variance of the First Passage Time

In analogy to the computation of the mean of the first passage time, we now calculate the second moment of the first passage time by solving

$$(i_0 - \sin(\varphi)) \frac{dT_2(\varphi \rightarrow \beta)}{d\varphi} + D \frac{d^2 T_2(\varphi \rightarrow \beta)}{d\varphi^2} = -2T_1(\varphi \rightarrow \beta)$$

(see [subsection 8.4.1](#)). One boundary condition is  $T_2(\varphi = \beta \rightarrow \beta) = 0$  (see [Equation 155](#)). The second boundary condition is  $T_2(\varphi \rightarrow \beta) \geq 0$  for  $\varphi \leq \beta$ .

Substitute  $z = T_2'$ . This yields the ODE

$$\frac{dz}{d\varphi} + \frac{i_0 - \sin(\varphi)}{D} z = -\frac{2}{D} T_1(\varphi \rightarrow \beta)$$

The general solution is

$$z(\varphi) = \exp\left(-\frac{i_0\varphi + \cos(\varphi)}{D}\right) \left( C_1 - \frac{2}{D} \int_{\beta}^{\varphi} T_1(\varphi'' \rightarrow \beta) \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' \right)$$

Integrating once yields the solution for  $T_2(\varphi \rightarrow \beta)$ :

$$\begin{aligned} T_2(\varphi \rightarrow \beta) &= \int_0^{\varphi} z(\varphi') d\varphi' \\ &= \int_{\beta}^{\varphi} \left[ \exp\left(-\frac{i_0\varphi' + \cos(\varphi')}{D}\right) \left( C_1 - \frac{2}{D} \int_{\beta}^{\varphi'} T_1(\varphi'' \rightarrow \beta) \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' \right) \right] d\varphi' \end{aligned}$$

From the boundary condition  $T_2((\varphi = \beta) \rightarrow \beta) = 0$ , we obtain that  $C_2 = 0$ .

From the condition that  $T_2(\varphi \rightarrow \beta) \geq 0$  for  $\varphi \leq \beta$ , we can derive a constraint for  $C_1$ :

$$\int_{\beta}^{\varphi} \left[ \exp\left(-\frac{i_0\varphi' + \cos(\varphi')}{D}\right) \left( C_1 - \frac{2}{D} \int_{\beta}^{\varphi'} T_1(\varphi'' \rightarrow \beta) \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' \right) \right] d\varphi' \geq 0 \quad \text{for all } \varphi$$

Flipping the integral boundaries on the outer integral and flipping signs on the inner integrand preserves the sign of the entire term:

$$\int_{\varphi}^{\beta} \left[ \exp\left(-\frac{i_0\varphi' + \cos(\varphi')}{D}\right) \left( -C_1 - \frac{2}{D} \int_{\varphi'}^{\beta} T_1(\varphi'' \rightarrow \beta) \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' \right) \right] d\varphi' \geq 0 \quad \text{for all } \varphi$$

The first exponential term is always  $\geq 0$ . This puts the constraint on the inner term:

$$-\frac{2}{D} \int_{\varphi'}^{\beta} T_1(\varphi'' \rightarrow \beta) \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' \geq C_1 \quad \text{for all } \varphi' \leq \beta$$

Since the integrand is always  $\geq 0$ , the integral is ever-decreasing for decreasing  $\varphi'$ . This means that the only  $C_1$  that fulfills this constraint is

$$C_1 = -\frac{2}{D} \int_{-\infty}^{\beta} T_1(\varphi'' \rightarrow \beta) \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi''$$

Substituting back and flipping the integration boundaries in the outer integral:

$$\begin{aligned}
T_2(\varphi \rightarrow \beta) &= \int_{\varphi}^{\beta} \left[ \exp\left(-\frac{i_0\varphi' + \cos(\varphi')}{D}\right) \right. \\
&\quad \left( \frac{2}{D} \int_{-\infty}^{\beta} T_1(\varphi'' \rightarrow \beta) \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' + \frac{1}{D} \int_{\beta}^{\varphi'} T_1(\varphi'' \rightarrow \beta) \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' \right) \\
&= \frac{2}{D} \int_{\varphi}^{\beta} \left[ \exp\left(-\frac{i_0\varphi' + \cos(\varphi')}{D}\right) \int_{-\infty}^{\varphi'} T_1(\varphi'' \rightarrow \beta) \exp\left(\frac{i_0\varphi'' + \cos(\varphi'')}{D}\right) d\varphi'' \right] d\varphi'
\end{aligned}$$

## 9 Overdamped RSJ Model (with noise): Other Solution Approaches

### 9.1 Moment Generating Function Approach

Using Ito's lemma (see [subsection 1.7](#)), the  $n$ -th moment's total differential is

$$\begin{aligned}\langle d\varphi^n \rangle &= \left\langle \left( \frac{\partial \varphi^n}{\partial t} + \nabla \varphi^n \cdot (i_0 - \sin(\varphi)) + D \nabla^2 \varphi^n \right) dt + \left( \nabla \varphi^n \cdot \sqrt{2D} \right) d\mathbf{w} \right\rangle \\ &= \left\langle ni_0 \varphi^{n-1} - \sum_{k=0}^{\infty} \frac{(-1)^k n}{(2k+1)!} \varphi^{2k+n} + Dn(n-1) \varphi^{n-2} \right\rangle d\tau\end{aligned}$$

This allows us to write the time-evolution of the  $n$ -th moment as

$$\frac{d}{d\tau} \langle \varphi^n \rangle = ni_0 \langle \varphi^{n-1} \rangle - \sum_{k=0}^{\infty} \frac{(-1)^k n}{(2k+1)!} \langle \varphi^{2k+n} \rangle + Dn(n-1) \langle \varphi^{n-2} \rangle$$

Define the moments  $\langle \varphi^n \rangle =: m_n$ :

$$\begin{aligned}m_0 &= 1 \\ \dot{m}_1 &= i_0 m_0 - \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} m_{2k+1} \\ \dot{m}_2 &= 2i_0 m_1 - \sum_{k=0}^{\infty} \frac{2(-1)^k}{(2k+1)!} m_{2k+2} + 2Dm_0 \\ \dot{m}_n &= ni_0 m_{n-1} - \sum_{k=0}^{\infty} \frac{(-1)^k n}{(2k+1)!} m_{2k+n} + Dn(n-1) m_{n-2}\end{aligned}$$

We define the moment-generating function (MGF) as:

$$M(t, s) = \sum_{n=0}^{\infty} \frac{m_n(t)}{n!} s^n, \quad (157)$$

which encodes all moments in a power series expansion. The moments can be recovered through differentiation:

$$m_n(t) = \left. \frac{\partial^n M(t, s)}{\partial s^n} \right|_{s=0}. \quad (158)$$

To derive the partial differential equation governing  $M(t, s)$ , we consider the time derivative:

$$\frac{\partial G}{\partial t} = \sum_{n=1}^{\infty} \dot{m}_n \frac{s^n}{n!}. \quad (159)$$

Substituting the moment equations: First Term ( $ni_0 m_{n-1}$ ):

$$\sum_{n=1}^{\infty} ni_0 m_{n-1} \frac{s^n}{n!} = i_0 s \sum_{n=1}^{\infty} m_{n-1} \frac{s^{n-1}}{(n-1)!} = i_0 s M(t, s). \quad (160)$$



Second Term (Sum over  $k$ ):

$$- \sum_{n=1}^{\infty} \sum_{k=0}^{\infty} \frac{(-1)^k n}{(2k+1)!} m_{2k+n} \frac{s^n}{n!} \quad (161)$$

$$= -s \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} \sum_{n=0}^{\infty} m_{2k+n+1} \frac{s^n}{n!} \quad (162)$$

$$= -s \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} \frac{\partial^{2k+1} G}{\partial s^{2k+1}} \quad (163)$$

$$= -s \sin \left( \frac{\partial}{\partial s} \right) M(t, s). \quad (164)$$

Third Term ( $Dn(n-1)m_{n-2}$ ):

$$D \sum_{n=2}^{\infty} n(n-1) m_{n-2} \frac{s^n}{n!} = Ds^2 \sum_{n=2}^{\infty} m_{n-2} \frac{s^{n-2}}{(n-2)!} = Ds^2 M(t, s). \quad (165)$$

Combining all terms, we obtain the evolution equation for the generating function:

$$\frac{\partial G}{\partial t} = i_0 s M(t, s) - s \sin \left( \frac{\partial}{\partial s} \right) M(t, s) + Ds^2 M(t, s) \quad (166)$$

$\sin \left( \frac{\partial}{\partial s} \right)$  is defined through its Taylor series expansion:

$$\sin \left( \frac{\partial}{\partial s} \right) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} \frac{\partial^{2k+1}}{\partial s^{2k+1}} \quad (167)$$

The Fourier transform of this term is

$$\mathcal{F} \left[ s \sin \left( \frac{\partial}{\partial s} \right) M(t, s) \right] = i \frac{\partial}{\partial \xi} \left[ \mathcal{F} \left( \sin \left( \frac{\partial}{\partial s} \right) M(t, s) \right) \right] \quad (168)$$

$$= i \frac{\partial}{\partial \omega} \left[ i \sinh(\omega) \tilde{G}(t, \omega) \right] \quad (169)$$

$$= -\frac{\partial}{\partial \omega} \left[ \sinh(\omega) \tilde{G}(t, \omega) \right] \quad (170)$$

The complete PDE in Fourier space becomes:

$$\frac{\partial \tilde{G}}{\partial t} = -i_0 \frac{\partial \tilde{G}}{\partial \omega} + \frac{\partial}{\partial \omega} \left[ \sinh(\omega) \tilde{G} \right] - D \frac{\partial^2 \tilde{G}}{\partial \omega^2} \quad (171)$$

Looks almost like Fokker-Planck all over again.

## 9.2 Rescaled Cumulant Generating Function Approach

$$M(k, \tau) = \langle e^{k\varphi} \rangle = \int e^{k\varphi} P(\varphi, \tau) d\varphi, \quad (172)$$

and the cumulant generating function (CGF) is its logarithm:

$$K(k, \tau) = \ln M(k, \tau). \quad (173)$$

Taking the time derivative of  $M(k, \tau)$ :

$$\frac{\partial M}{\partial \tau} = \int e^{k\varphi} \frac{\partial P}{\partial \tau} d\varphi. \quad (174)$$

Substituting the Fokker-Planck equation:

$$\frac{\partial M}{\partial \tau} = \int e^{k\varphi} \left( -\frac{\partial}{\partial \varphi} [(i_0 - \sin \varphi)P] + D \frac{\partial^2 P}{\partial \varphi^2} \right) d\varphi. \quad (175)$$

For the drift term (partial integration and vanishing at boundaries):

$$\int e^{k\varphi} \left( -\frac{\partial}{\partial \varphi} [(i_0 - \sin \varphi)P] \right) d\varphi = \int [(i_0 - \sin \varphi)P] \frac{\partial}{\partial \varphi} e^{k\varphi} d\varphi \quad (176)$$

$$= k \langle (i_0 - \sin \varphi) e^{k\varphi} \rangle. \quad (177)$$

For the diffusion term (twice partial integration and vanishing at the boundaries):

$$D \int e^{k\varphi} \frac{\partial^2 P}{\partial \varphi^2} d\varphi = D k^2 M(k, \tau). \quad (178)$$

The time evolution of the MGF becomes:

$$\frac{\partial M}{\partial \tau} = k \langle (i_0 - \sin \varphi) e^{k\varphi} \rangle + D k^2 M. \quad (179)$$

Dividing by  $M$  gives the CGF equation:

$$\frac{1}{M} \frac{\partial M}{\partial \tau} = \frac{\partial K}{\partial \tau} = k i_0 + D k^2 - k \frac{\langle \sin \varphi e^{k\varphi} \rangle}{M}. \quad (180)$$

Expressing  $\sin \varphi$  using exponentials:

$$\sin \varphi = \frac{e^{i\varphi} - e^{-i\varphi}}{2i}, \quad (181)$$

we have:

$$\langle \sin \varphi e^{k\varphi} \rangle = \frac{e^{K(k+i)} - e^{K(k-i)}}{2i} M(k, \tau). \quad (182)$$

Substituting back yields a PDE for the CGF:

$$\boxed{\frac{\partial K}{\partial \tau} = k i_0 + D k^2 - \frac{k}{2i} (e^{K(k+i)-K(k)} - e^{K(k-i)-K(k)})}. \quad (183)$$

Rescale all cumulants by  $1/\tau$ :

$$\tilde{\kappa}_n(\tau) = \frac{\kappa_n(\tau)}{\tau} \quad (184)$$

This gives the rescaled CGF:

$$\tilde{K}(k, \tau) = \sum_{n=1}^{\infty} \frac{k^n}{n!} \tilde{\kappa}_n(\tau) = \frac{K(k, \tau)}{\tau} \quad (185)$$

Compute the time derivative:

$$\frac{\partial \tilde{K}}{\partial \tau} = \frac{\partial}{\partial \tau} \left( \frac{K}{\tau} \right) = \frac{1}{\tau} \frac{\partial K}{\partial \tau} - \frac{K}{\tau^2} \quad (186)$$

Substitute the original CGF equation:

$$\tau \frac{\partial \tilde{K}}{\partial \tau} + \tilde{K} = ki_0 + Dk^2 - \frac{k}{2i} \left( e^{\tau(\tilde{K}(k+i) - \tilde{K}(k))} - e^{\tau(\tilde{K}(k-i) - \tilde{K}(k))} \right) \quad (187)$$

One can show that for bounded drift and constant diffusion, all cumulants scale at most linearly for  $\tau \rightarrow \infty$ . Weirdly enough, this would yield that in the long time limit, velocity and variance scale like  $\sim i_0 \tau$  and  $\sim 2D\tau$ , which is wrong.

## 10 Overdamped RSJ model: TUR

Recalling Equation 151:

$$\lim_{\tau \rightarrow \infty} \frac{\langle \varphi(\tau) \rangle}{\tau} = \lim_{\tau \rightarrow \infty} \frac{2\pi \langle N(\tau) \rangle}{\tau} = \frac{2\pi}{\mu} \quad (188)$$

$$\lim_{\tau \rightarrow \infty} \frac{\langle \langle \varphi^2(\tau) \rangle \rangle}{\tau} = \lim_{\tau \rightarrow \infty} (2\pi)^2 \frac{\langle \langle N^2(\tau) \rangle \rangle}{\tau} = (2\pi)^2 \frac{\sigma^2}{\mu^3} \quad (189)$$

where  $\mu = T_1(0 \rightarrow 2\pi)$  and  $\sigma^2 = T_2(0 \rightarrow 2\pi) - T_1^2(0 \rightarrow 2\pi)$  The entropy production is

$$\sigma t = \bar{V} I_0 = \langle \bar{\dot{\varphi}} \rangle \frac{\phi_0}{t_0} i_0 I_c \tau t_0 = \langle \bar{\dot{\varphi}} \rangle i_0 \phi_0 I_c = \langle \bar{\dot{\varphi}} \rangle i_0 \frac{\hbar I_c}{2e}$$

Then, the LHS of the TUR is given by

$$\frac{\langle \langle \varphi^2(\tau) \rangle \rangle}{\langle \varphi(\tau) \rangle^2} \sigma \tau = \frac{T_2(0 \rightarrow 2\pi) - T_1^2(0 \rightarrow 2\pi)}{T_1^3(0 \rightarrow 2\pi)} T_1^2(0 \rightarrow 2\pi) \langle \bar{\dot{\varphi}} \rangle i_0 = 2\pi \left( \frac{T_2(0 \rightarrow 2\pi)}{T_1^2(0 \rightarrow 2\pi)} - 1 \right)$$

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