PHY2705. Stochastic Processes. Lecture Notes.

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Chapter 1

Introduction. Probabilistic descriptions of stochastic processes. Master equation and its approximations.

1.1 Random walks on a lattice.

1.1.1 Symmetric random walk.

The probability of a one-dimensional random walker to go distance n in N steps is proportional to the number of walks that lead to n in N steps, that is to the number of ways to make $N_\rightarrow$ steps to the right and $N_\leftarrow$ steps to the left, so that $n = N_\rightarrow - N_\leftarrow$. This number is

$$M(n,N) = \frac{N!}{N_\rightarrow! N_\leftarrow!} = \frac{N!}{\frac{(N-n)}{2}! \frac{(N+n)}{2}!}. \tag{1.1}$$

Note that $\sum_{n=0}^{N} M(N,n) = 2^N$, so that the *probability* to be at n at time N is:

$$P(n,N) = \frac{M(N,n)}{2^N} \tag{1.2}$$

We calculate an approximation to $P(n,N)$, using *Stirling approximation:* $\ln(N!) \simeq N \ln N - N +$

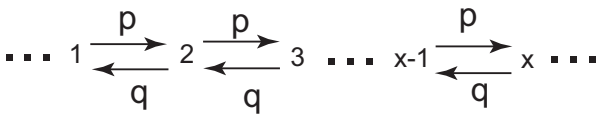

Figure 1.1: Random walk in one dimension. p and q are the probabilities of jumping either left or right. In the symmetric case considered here, $p = q = 1/2$

$\frac{1}{2}\ln(2\pi N)$. Then

$$\begin{aligned}\ln P(n,N) &= -N\ln 2 + N(\ln N - 1) + \frac{1}{2}\ln(2\pi N) - \frac{1}{2}(N+n)(\ln(\frac{N+n}{2}) - 1) \\ &- \frac{1}{2}\ln(2\pi(N+n)/2) - \frac{1}{2}(N-n)(\ln(\frac{N-n}{2}) - 1) - \frac{1}{2}\ln(2\pi(N-n)/2) \\ &= -\frac{N}{2}\left[(1+n/N)\ln(1+n/N) + (1-n/N)\ln(1-n/N)\right] - \frac{1}{2}\ln(2\pi N) \\ &- \frac{1}{2}\ln((1+n/N)(1-n/N)) + \ln 2 \end{aligned} \tag{1.3}$$

Expanding up to second order in n and collecting the terms, we get:

$$\ln P(n,N) = -n^2/(2N) + \ln(2/\sqrt{2\pi N}) \tag{1.4}$$

or

$$P(n,N) = \frac{2}{\sqrt{2\pi N}}\exp\left(-\frac{n^2}{2N}\right) \tag{1.5}$$

We can convert the discrete probability $P(n,N)$ into a continuous probability density $P(r,t)$ in the continuum limit ($a \to 0$, $\tau \to 0$), where $r = na$ and $t = N\tau$). Then

$$P(r,t)dr = P(n,N)dr/(2a) = \frac{1}{a\sqrt{2\pi t/\tau}}\exp\left(-\frac{n^2\tau}{2a^2 t}\right)dr = \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{r^2}{4Dt}\right)dr \tag{1.6}$$

The constant $D = \frac{a^2}{2\tau}$ is called *diffusion coefficient* for reasons that will become apparent later. (See Phillips textbook section **8.2**). Averaging over the ensemble of identical random walks, we get:

$$\begin{aligned}\langle r\rangle &= \int_{-\infty}^{\infty} rP(r,t)dr = 0 \\ \langle r^2\rangle(t) &= \int_{-\infty}^{\infty} r^2 P(r,t)dr = 2Dt \end{aligned} \tag{1.7}$$

Analogously, in the original discrete formulation:

$$\langle n^2\rangle(N) = \sum_n n^2 P(n,N) = N \tag{1.8}$$

That is, the mean square displacement of a random walker scales like $t^{1/2}$ - very different from Newtonian motion on the macroscale.

Central limit theorem, aka the Strong Law of Large Numbers Statement: if we have N identically distributed random variables $x_1, ...x_i, ...x_N$ then, no matter what is the distribution, the random variable $X = \sum_{i=1}^{N} x_i$ has a Gaussian (Normal) distribution with the mean $N\langle x\rangle$ and variance $N(\langle x^2\rangle - \langle x\rangle^2)$ (**Off-line:** read any book in probability theory for proof).

1.1.2 Random walk with constant bias.

Consider a more complicated case when the random walk is not symmetric, so that the probability to jump to the right is q and the probability to jump to the left is $q = 1 - p$. For convenience, we define $\epsilon = p - q$ as a measure of bias, so that $q = (1-\epsilon)/2$ and $p = (1+\epsilon)/2$.

From general considerations of the Central Limit Theorem, we can guess that the probability distribution of such random walker $P(x,t)$ is going to be Gaussian. The mean of this distribution can be calculated as

follows. The position r after N steps (time t) is $x(t) = \sum_{i=1}^{N} \Delta x_i$ where Δx_i is an individual step (forward or backward in the one-dimensional case); note that here $x(t)$ is a *random variable*. Thus,

$$\langle x(t) \rangle = \sum_{i=1}^{N} \langle \Delta x_i \rangle = Na(p-q) \tag{1.9}$$

because $\langle \Delta x_i \rangle = a(p-q)$.

The second moment is

$$\langle x(t)^2 \rangle = \langle \sum_{i=1}^{N} \Delta x_i \sum_{j=1}^{N} \Delta x_j \rangle = N \sum_{i=1}^{N} \langle (\Delta x_i)^2 \rangle + \sum_{i \neq j} \langle \Delta x_i \Delta x_j \rangle = Na^2 + N(N-1)a^2(q-p)^2$$

because $\langle (\Delta x_i)^2 \rangle = a^2(p+q) = a^2$

After some algebra, we can calculate the variance

$$\langle r^2 \rangle - \langle r \rangle^2 = 4Na^2pq = Na^2(1-\epsilon^2) = 2Dt(1-\epsilon^2) \tag{1.10}$$

1.1.3 Fokker-Planck equation with constant bias.

The equation for the probability is:

$$P(x, t+\tau) = qP(x+a, t) + pP(x-a, t) \tag{1.11}$$

Expanding again to the second order in a and first order in τ, we get:

$$\frac{\partial}{\partial t} P(x,t) = \frac{a^2}{2\tau} \frac{\partial^2}{\partial x^2} P(x,t) + \frac{a}{\tau}(q-p) \frac{\partial}{\partial x} P(x,t) = -\frac{\partial}{\partial x} J(x) \tag{1.12}$$

with $J(x) = \frac{a}{\tau}(p-q)P(x,t) - \frac{a^2}{2\tau}\frac{\partial}{\partial x}P(x,t)$.

1.1.4 Spatially varying hopping rates.

The derivations change only slightly if the hopping probabilities are not constant, but depend on the position x: $p(x)$ and $q(x)$. The Master equation then reads:

$$P(x,t) = p(x+a)P(x+a, t-\tau) + q(x-a)P(x-a, t-\tau) \tag{1.13}$$

Expanding the p and q up to the second order in a as well, $p(x \pm a) = p(r) \pm ap'(x) + \frac{1}{2}a^2p''(x)$, and doing all the algebra, we get:

$$\frac{\partial}{\partial t} P(x,t) = \frac{a^2}{2\tau} \frac{\partial^2}{\partial x^2} P(x,t) + \frac{a}{\tau} \frac{\partial}{\partial x} \left[(-p(x) + q(x)) P(x,t) \right] = -\frac{\partial}{\partial x} J(x) \tag{1.14}$$

with $J(x) = \frac{a}{\tau}(p(x) - q(x))P(x,t) - \frac{a^2}{2\tau}\frac{\partial}{\partial x}P(x,t)$. See class notes for algebra details. This is the Fokker-Planck equation for the above random walk (Master) equation.

1.1.5 Equilibrium

If $p(x)$ and $q(x)$ are arising from action of a certain potential $U(x)$, the equilibrium considerations place powerful constraints.

At equilibrium, the flux through the system $J(x) = 0$ is zero. That is

$$\frac{a}{\tau}(p(x) - q(x))P(x,t) - \frac{a^2}{2\tau}\frac{\partial P(x,t)}{\partial x} = 0 \tag{1.15}$$

Defining $p(x) - q(x) = \epsilon(x)$ as above, this equation has a solution

$$P^{\text{eq}}(x) \simeq \exp\left(\frac{2}{a}\int^x dx'\epsilon(x')\right) \tag{1.16}$$

The equilibrium probability $P^{\text{eq}}(x)$ has to obey the Boltzmann distribution $P^{\text{eq}}(x) \simeq \exp(-U(x)/kT)$. Thus

$$\epsilon(x) = -\frac{a}{2kT}\frac{\partial U(x)}{\partial x} = \frac{a}{2kT}F(x)$$

.

Finally, the above Fokker-Planck equation becomes

$$\frac{\partial}{\partial t}P(x,t) = D\frac{\partial^2}{\partial x^2}P(x,t) + \frac{D}{kT}\frac{\partial}{\partial x}U(x)\frac{\partial}{\partial x}P(x,t) \tag{1.17}$$

Or, in other words

$$\frac{\partial}{\partial t}P(x,t) = -\frac{\partial J(x,t)}{\partial x} \tag{1.18}$$

with the flux

$$J(x,t) = -D\frac{\partial P(x,t)}{\partial x} + \frac{D}{kT}F(x)P(x) \tag{1.19}$$

In this form, it is known as the *Smoluchowski equation*.

1.1.6 First moment and variance

Unlike the unbiased diffusion, the mean displacement $\langle r\rangle$ is not zero. Lets calculate he first moment and the variance from the Smoluchowski equation for constant $p(x) = p$ and $q(x) = q$ and compare them to the results obtained by direct summation in the beginning of this chapter.

We can calculate it using the following mathematical trick:

$$\begin{aligned}
\frac{d}{dt}\langle x\rangle(t) &= \int_{-\infty}^{\infty} dx x\frac{\partial}{\partial x}P(x,t) = \\
&= \int_{-\infty}^{\infty} dx x\frac{\partial}{\partial x}\left(D\frac{\partial P(x,t)}{\partial x} + \frac{a}{\tau}(q-p)P(x,t)\right) = \\
&= r\left(D\frac{\partial P(x,t)}{\partial x} + \frac{a}{\tau}(q-p)P(x,t)\right)|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} dx\left(D\frac{\partial}{\partial x}P(x,t) + \frac{a}{\tau}(q-p)P(x,t)\right) \\
&= DP(r,t)|_{-\infty}^{\infty} - \frac{a}{\tau}(q-p)\int dx P(x,t) = \frac{a}{\tau}(p-q)
\end{aligned} \tag{1.20}$$

where we have used the fact that the probability density $P(x,t)$ decays faster than $1/x$ at $x \to \pm\infty$ (otherwise, it is non-normalizable) and that $\int dx P(x,t) = 1$ for any t.

Therefore

$$\frac{d}{dt}\langle r\rangle(t) = \frac{a}{\tau}(p-q) \quad \text{or} \quad \langle x\rangle(t) = \frac{a}{\tau}\epsilon t$$

Substituting $\epsilon = \frac{a}{2\tau kT}F$, we finally get:

$$\langle x\rangle(t) = \mu F t$$

with $\mu = \frac{D}{kT}$. This is known as Einstein relation, and is a special case of a more general fluctuation-dissipation theorem.

Thus, the first moment of the distribution agrees with the direct summation method above. The second moment and the variance, $\langle x^2\rangle - \langle x\rangle^2$ can be using the same trick, which is left as a homework.

1.1.7 Deterministic limit for single particle motion.

Within the derivation above, the mean $\langle x\rangle(t)$ has a meaning only as an ensemble average over many particles. Each individual particle within that ensemble performs a random trajectory, and its position at any given time can be quite far from the ensemble mean. Nevertheless, it is clear that as the bias $p-q$ increases, the motion becomes more and more deterministic - indeed when $p = 1$ the particle moves deterministically to the right at each step. This is reflected in the fact that $\langle (x - \langle x\rangle)^2\rangle(t) = 2Dt(1-\epsilon^2)$. So, in the regime where $\frac{Ft(Dt)^{1/2}}{kT} \gg (2(1-\epsilon^2)^{1/2}$, behavior of each particle becomes almost deterministic [Show the evolution of the distribution in time].

In this regime, one can speak of the velocity of one particle: $v = \frac{DF}{kT}$. As one might recall, similar behavior arises in a different system - Stokes drag on a particle immersed in a fluid [Show the Stokes law and the diagram]. The reason is that the random walk and the viscosity come from the same molecular source - collisions with the molecules of the surrounding fluid. This will lead to the discussion of the Langevin formalism in the next section. **Illustrations (see class slides): Meselson-Stahl experiment. Stokes law from macroscopic to molecular scales**

1.2 Random walk with exponentially distributed jump times: the standard form of the Master equation.

Probability distribution of times between jumps is $\rho(a) = (r^p + r^q)e^{-(r^p+r^q)a}$. Probability to jump forward in a small interval Δt is $r^p\Delta t$ and $r^q\Delta t$ respectively for jumping backward. Then the probability of *not* jumping by time t, $P_0(t)$, can be derived by integrating the expression (a):

$$P_0(a+da) = P_0(a)(1-(r^p+r^q)da)$$

, which gives $P_0(t) = \exp(-(r^p+r^q))$

Thus

$$P_i(t+\Delta t) = P_i(t)(1-(r_i^p+r_i^q)\Delta t) + P_{i+1}r_{i+1}^q\Delta t + P_{i-1}r_{i-1}^p\Delta t \tag{1.21}$$

at each site, the *probability* of eventually jumping to the right is $p = \frac{r^p}{r^p+r^q}$. After *defining* $r^p = p/\tau$ and $r^q = q/\tau$, the above equation becomes

$$\frac{P_i(t+\Delta t) - P_i(t)}{\Delta t} = r_{i-1}^p P_{i-1}(t) + r_{i+1}^q P_{i+1}(t) + P_i(t) \tag{1.22}$$

This is the *standard form* of the Master equation. It can be also Taylor expanded as before to get to the Fokker-Planck equation. It can be generalized to an arbitrary Markov process with any connectivity diagram given by a matrix $\hat{M}$:

$$\frac{d\vec{P}}{dt} = \hat{M}\cdot\vec{P}(t)$$

where $\vec{P}(t) = (P_1(t), P_2(t), ..., P_i(t)$ and $M_{ij} = r_{ji}(1-\delta_{ij}) - \delta_{ij}\sum_{j'} r_{ij'}$.

1.2.1 Detailed balance, steady state and equilibrium

. Master equation has to conserve probability, $\sum_i P_i(t) = 1$,at all times. This has important consequences:

$$\frac{d}{dt}\sum_i P_i(t) = \sum_i \sum_j M_{ij}P_j(t) = \sum_j (\sum_i M_{ij})P_j(t) = 0 \tag{1.23}$$

Therefore, $\sum_i M_{ij} = 0$ for all j - the sum of the matrix elements in every column is zero. Thus, matrix $\hat{M}$ is degenerate, and its determinant is $\text{Det}(\hat{M}) = 0$, implying that at least one of the eigenvalues of $\hat{M}$ is zero. Thus, any Markov process possesses at least one steady state, where $\frac{d\vec{P^{ss}}}{dt} = \hat{M}\cdot\vec{P}^{ss} = 0$.

Equilibrium is a very special case of a steady state where the mean flux between any two states is zero, so that $P_i^{eq} r_{ij} = P_j^{eq} r_{ji}$. If this condition is satisfied for all pairs of i and j, the system is said to be in *detailed balance*.

On the other hand, we know that the equilibrium distribution is the Boltzmann distribution, $P_i^{eq} = e^{-E_i/kT}/\sum_j e^{-E_j/kT}$ and therefore $r_{ij}/r_{ji} = \exp(-(E_j - E_i)/kT)$. This condition is equivalent to the statement that in every loop in the state space, the product of the rates counterclockwise is equal to the product of the rates in the clockwise direction. This is known as *detailed balance condition* in physics or Kolmogorov condition in mathematics.

1.3 Randomly distributed jump lengths: Einstein formulation

Consider a case when the jump time τ is fixed but the jump distance l obeys some probability distribution $g(l)$, which can depend on the position x, $g(x,l)$. Then the probability to be at a position x at time $t+\tau$ is

$$P(x, t+\tau) = \int dx' P(x', t) g(x, x-x') = \int dz P(x-z, t) g(x-z, z) \tag{1.24}$$

where $z = x - x'$. Expanding $P(x, t+\tau) = P(x,t) + \tau\frac{\partial P}{\partial t}$ and $P(x-z,t)g(x-z,z) = P(x,t) - z\frac{\partial P(x,t)g(x,z)}{\partial x} + \frac{1}{2}z^2\frac{\partial^2 P(x,t)g(x,z)}{\partial x^2}$, we get

$$\tau\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}P(x,t)\int dz z g(x,z) + \frac{1}{2}\frac{\partial^2}{\partial x^2}P(x,t)\int dz z^2 g(x,z) \tag{1.25}$$

Denoting $A(x) = \frac{1}{\tau}\int dz z g(x,z)$ and $B(x) = \frac{1}{2\tau}\int dz z^2 g(x,z)$ it becomes

$$\tau\frac{\partial P}{\partial t} = -\frac{\partial P(x,t)A(x)}{\partial x} + \frac{1}{2}\frac{\partial^2 P(x,t)B(x)}{\partial x^2} \tag{1.26}$$

When B is independent of x it becomes the Smoluchowski equation if one identifies $A(x) = (p(x) - q(x))a$. We will return to the case of $B(x)$ explicitly depending on x later.

1.4 Langevin equation

For one particle in the limit of large force,

$$\dot{x}(t) = \mu(F(x) + \xi(t)) \tag{1.27}$$

where $\xi(t)$ is a random force. Note that in this formulation $x(t)$ is a *random variable*. The random force $\xi(t)$ is a gaussian white noise with the mean $\langle \xi(t) \rangle = 0$ for all t and $\langle \xi(t)\xi(t') \rangle = \Gamma \delta(t-t')$. What this means is that at each time step t, the value of the corresponding ξ is chosen from a gaussian distribution with zero mean and variance Γ: $P(\xi) \simeq \exp(-\frac{\xi^2}{2\Gamma})$. Mathematically, the probability of the time course of $\xi(t)$ is

$$P(\xi(t)) = \frac{\exp(-\frac{1}{2\Gamma}\int_0^t dt' \xi(t')^2)}{\int D\xi(t) \exp(-\frac{1}{2\Gamma}\int_0^t dt' \xi(t')^2}$$

.

1.4.1 First and second moment of $x(t)$: comparison to the Fokker-Planck and the Master equation.

Mean (assuming $x(0) = 0$):

$$\langle x(t) \rangle = \mu \int_0^t dt' (F + \langle \xi(t') \rangle) = \mu F t \tag{1.28}$$

Second moment:

$$\begin{aligned} \langle x^2(t) \rangle &= \langle (\mu \int_0^t dt' (F + \xi(t'))^2 \rangle \\ &= \mu^2 F^2 t^2 + \int_0^t dt' \int_0^t dt'' \langle \xi(t')\xi(t'') \rangle \\ &= \mu^2 F^2 t^2 + \mu^2 \int_0^t dt' \int_0^t dt'' \Gamma \delta(t'-t'') = \mu^2 F^2 t^2 + \Gamma t \end{aligned}$$

Variance:

$$\langle x^2(t) \rangle - \langle x(t) \rangle^2 = \mu^2 \Gamma t \tag{1.29}$$

Identifying $mu^2\Gamma = 2D$, and using the Einstein Relation $D = \mu k T$, we get $\Gamma = 2kT/\mu$. This agrees with the direct summation result for $F = 0$. However, it is missing a factor $1-\epsilon^2$ form $F \neq 0$. This is because the Fokker-Planck approximation is not a true continuum limit, but an expansion, also known as Kramers-Moyal expansion. The issue lies in the way a and τ tend to zero. In order that the diffusion coefficient D stays constant $a^2 \sim \tau$ in the limit $a, \tau \to 0$. This means that the drift term, which has a prefactor $a\epsilon/\tau \sim \epsilon/a$, diverges unless $\epsilon \to 0$ as well. So, the Fokker-Planck/Smoluchowski is consistent only in the limit of small biad/force. The situation can be remedies by considering higher terms in the expansion in the powers of τ (see notes on Kramers-Moyal expansion on the wiki).

1.4.2 Equivalence of the Langevin and Fokker-Planck formulation: $P(x,t)$.

We first show that for $F = 0$ the Langevin equation produces the same $P(x,t)$ as the Fokker-Planck or direct summation.

Mathematically, $P(z,t) = \langle \delta(x(t) - z) \rangle_{\{\xi(t)\}}$ where the average is over all realizations of $\xi(t)$.

Auxiliary. First, let us prove some helpful mathematical identities. First,

$$\int_{-\infty}^{\infty} dz \exp(az - \frac{z^2}{2b}) / \int_{-\infty}^{\infty} dz \exp(-\frac{z^2}{2b}) = \exp(ba^2/2) \tag{1.30}$$

and

$$\langle \exp(c \int_0^t \xi(t') dt') \rangle_{\{\xi(t)\}} = \exp(c^2 \Gamma t/2) \tag{1.31}$$

PROOF: Discretizing the interval $[0,t]$ into n small bins of length τ each:

$$\begin{aligned}\langle \exp(c\int_0^t \xi(t')dt')\rangle_{\{\xi(t)\}} &= \frac{\int \prod_i^n d\xi_i \exp(c\tau\sum_{i=1}^n \xi_i - \tau\sum_i \frac{\xi_i^2}{2\Gamma}))}{\int \prod_i d\xi_i \exp(-\tau\frac{\xi_i^2}{2\Gamma})} \\ &= \frac{\prod_i^n \int d\xi_i \exp(\tau(c\sum_i^n \xi_i - \frac{\xi_i^2}{2\Gamma}))}{\prod_i^n \int d\xi_i \exp(-\tau\frac{\xi_i^2}{2\Gamma})} \\ &= \prod_i^n \exp(\tau c^2\Gamma/2) = \exp(c^2\tau n/2) = \exp(c^2\Gamma t/2)\end{aligned}$$

Thus,

$$\begin{aligned}P(z,t) &= \frac{1}{2\pi}\int dk \langle \exp(ik(\mu\int_0^t \xi(t')dt' - z)\rangle_\xi \\ &= \tfrac{1}{2\pi} \int dk \exp(-ikz)\exp(-k^2\mu^2\Gamma t/2) = \exp(-z^2/(4Dt))/(4\pi Dt)^{1/2} \end{aligned} \quad (1.32)$$

where we have used the fact that $D = \mu^2\Gamma/2$ and $D = \mu kT$.

More direct proof.

One could also observe that

$$\begin{aligned}\frac{\partial P(z,t)}{\partial t} &= \partial_t \int dk \langle \exp(ik\mu\int_0^t dt'\xi(t') - z)\rangle_\xi = \int dk \exp(-ikz)\partial_t \exp(-k^2\mu^2\Gamma t/2) \\ &= \int dk \frac{1}{2}(-k^2)\mu^2\Gamma \exp(-ikz)\exp(-k^2\mu^2\Gamma t/2) \end{aligned} \quad (1.33)$$

On the other hand,

$$\begin{aligned}\frac{\partial^2 P(z,t)}{\partial z^2} &= \int dk(-k^2\langle \exp(\mu\int_0^t dt'\xi(t') - z)\rangle_\xi = \\ &= \int dk(-k^2)\exp(-ikz)\exp(-k^2\mu^2\Gamma t/2) \end{aligned} \quad (1.34)$$

Recalling that $D = \mu^2\Gamma/2$, this leads to

$$\frac{\partial P(z,t)}{\partial t} = D\frac{\partial^2 P(z,t)}{\partial z^2}$$

.

General SDE-PF equivalence

For a continuous state variable the stochastic evolution of the system can be thought of as the deterministic motion with added random fluctuations. A familiar example of this case is the Langevin equation that describes the motion of a diffusing Brownian particle,

$$\dot{x}(t) = \mu(f(x) + \xi(t)), \quad (1.35)$$

where $f(x)$ is the deterministic force acting on the particle, ξ is a random force that mimics the effects of random jumps, and μ is the mobility. Note that $x(t)$ is now a *random variable*. The formal connection

between this representation and the probability density of the previous section is provided by the relation $p(s,t) = \langle \delta(x(t) - s) \rangle_\xi$, where the average is over all the realizations of the random force ξ.

It can be shown that with the choice of $\mu = D/kT$ and $\langle \xi(t)\xi(t') \rangle = \frac{kT}{D^{1/2}} \delta(t - t')$, this equation is mathematically equivalent to the following Fokker-Planck equation,

$$\partial_t p(s,t) = -\partial_s(\mu f(s) p(s,t)) + D\partial_s^2 p(s,t). \tag{1.36}$$

More generally, any Fokker-Planck equation of the form

$$\partial_t p(x,t) = -\partial_x \left(A(x)p(x,t)\right) + \frac{1}{2}\partial_x^2 \left(B(x)p(x,t)\right) \tag{1.37}$$

has an equivalent stochastic differential equation (SDE) of the form

$$\dot{x}(t) = A_0(x) + B_0(x)\chi(t), \tag{1.38}$$

with delta-correlated random term $\langle \chi(t)\chi(t') \rangle = \delta(t - t')$. However, due to mathematically pathological properties of the function $\chi(t)$ (it is nowhere differentiable), when $B_0(x)$ depends on x, the Eq. (1.38) is not un-ambiguosly defined. In general, its interpretation requires re-definition of the rules of differentiation and integration, and many different SDE's can be chosen to correspond to the same FPE, depending on the interpretation.

Historically, the two major interpretations are from Ito and Stratonovich. In both these formulations, $B_0(x) = B(x)^{\frac{1}{2}}$. However, $A_0(x) = A(x)$ in Ito interpretation while $A_0(x) = A(x) - \frac{1}{4}\partial_x B(x)$ in the Stratonovich interpretation. From the practical perspective, Ito interpretation allows the simulation of the SDE using the usual forward Euler scheme. However, special differentiation and integration rules are required for analytical calculations. On the other hand, Stratonovich interpretation allows using the regular rules of calculus but has to be simulated using implicit schemes. We emphasize that the Fokker-Planck equation does not suffer from such ambiguity of interpretation; SDEs corresponding to different interpretations of the same Fokker-Planck equation lead to the same physical result [NEED TO COMPLETE THIS SECTION FOR x-dependent $B(x)$]

1.4.3 Langevin with inertia.

The overdamped Langevin equation can be taken one step back to introduce the inertia in order to describe the transients and velocity fluctuations around the steady state solution. The Newton equation for a particle under an action of an external force F is:

$$m\ddot{x} = -\dot{x}/\mu + F + \xi \tag{1.39}$$

where the second term describes friction. At long times, the acceleration term becomes negligible, and we recover the overdamped steady state solution $v = \mu(F + \xi)$.

Let us look at the fluctuations of velocity $v = \dot{x}$ around the deterministic solution $v = 0$ in the absence of the external force. They then obey

$$m\dot{v} = -v/\mu + \xi \tag{1.40}$$

Using the method of multipliers, we get $v(t) = \frac{1}{m}\int_0^t dt' \xi(t') e^{-(t-t')/(m\mu)}$. And

$$\langle v(t)^2 \rangle = \frac{1}{m^2} e^{-2t/(m\mu)} \langle \int_0^t \int_0^t dt' dt'' e^{2t'/(m\mu)} \langle \xi(t')\xi(t'') \rangle = \frac{\Gamma\mu}{2m}(1 - e^{-2t/(m\mu)}) \tag{1.41}$$

Remembering that $\Gamma = 2kT/\mu$, we get that the average kinetic energy of the particle at time t is

$$\frac{1}{2}m\langle v(t)^2 \rangle = \frac{kT}{2}(1 - e^{-2t/(m\mu)}) \to \frac{kT}{2} \text{ when } t \to \infty \tag{1.42}$$

, which means that after the transients die out in a time $m\mu$, the velocity fluctuations around equilibrium are as expected from the equipartition theorem. Note that although our initial formulation of the random walk had no connection to any underlying molecular kinetics, due to the requirement that the steady state solution is Boltzmann distribution, the whole mathematical structure is consistent with statistical mechanics.

In principle, we could also write the full Fokker-Planck equation for the probability of a particle to be at a position x and have a velocity v, $P(x, v)$ that would correspond to the Langevin equation with inertia (see additional literature on the wiki).

1.5 Simulation methods.

1.5.1 Simulating Langevin equation: Wiener process

Langevin equation is the easy to simulate using Euler-like scheme:

$$x_{n+1} = x_n + \mu f(x_n)\Delta t + \Delta W \tag{1.43}$$

where ΔW is known as the *Wiener Process*. Although as a mathematical (random) function it has some pathological properties, in practice it is very easy to use: according to the previous section, $\Delta W = \int_0^{\Delta t} \xi(t')dt'$ is a Normally distributed random number with the mean equal to zero, and the variance equal $2kT/\mu\Delta t = 2D\Delta t$.

1.5.2 Simulating the Master equation: Gillespie-Kalos-Bortz-Leibowitz aka Kinetic Monte Carlo aka Stochastic Simulation algorithm.

Assume a stochastic process with N states enumerated with index i, with the transition rates r_{ij} from i to j. At each simulation step,if the system is at state i, generate partial sums $g_k = \sum_{j<k} r_{ji} / \sum_{j=1}^{N} r_{ji}$ for $k = 2$ to $k = N$. Generate a random number X uniformly distributed in the interval $[0, 1]$. If $g_{k-1} < X < g_k$ (which happens with probability $r_{ki} / \sum_{j=1}^{N} r_{ji}$, move the system into the appropriate state k. The probability distribution of the ensemble of resulting trajectories is the exact solution of the corresponding Master equation.

1.5.3 Simulating the Fokker-Planck equation.

The FP equation can be propagated in time using the Green function method:

$$P(x, t + \Delta t) = \int dx' G(x, x', \Delta t) P(x', t) \tag{1.44}$$

where the propagator $G(x, x', \Delta t)$ is the solution to the FP equation with the initial condition at x':

$$G(x, x', \Delta t) = \frac{1}{\sqrt{4\pi D\Delta t}} e^{\frac{-(x-x'-v(x')\Delta t)^2}{4D\Delta t}} \tag{1.45}$$

where $v(x) = \frac{D}{kT} f(x)$ is the instantaneous velocity of the distribution mean (See the section on the Fokker-Planck equation).

1.6 Path integral formulation.

An interesting perspective on the stochastic processes of continuous variable can be gleaned by casting them in the path integral formalism. The idea is the same as in quantum mechanics: we need to find a function

that describes the probability of a given trajectory $x(t)$. Then the probability of going from x_0 to x_f in time t is the appropriately weighted sum over all possible trajectories.

To simplify things, we start with the discrete formulation and take the continuous limit later. Then, the trajectory is defined as a sequence of positions $x_0, x_1(\Delta t), x_2(2\Delta t)...x_n(n\Delta t)...x_f(t)$; $t = N\Delta t$. The probability of going from x_{n-1} to x_n in Δt is

$$P(x_n, t+\Delta t|x_{n-1}, t) = \frac{1}{\sqrt{4\pi D\Delta t}} e^{-\frac{(x_{n+1}-x_n-\frac{Df(x_n)}{kT}\Delta t)^2}{4D\Delta t}} \tag{1.46}$$

Then the total probability is

$$\begin{aligned}
P(x_f, t|x_0, 0) &= \int \prod_{n=1}^{N-1} dx_n P(x_n, \Delta t + t_{n-1}|x_{n-1}, t_{n-1}) P(x_f, t|x_{N-1}, t_{N-1}) \\
&= \int \prod_{n=1}^{N-1} dx_n \frac{1}{\sqrt{4\pi D\Delta t}} e^{-\frac{(x_n-x_{n-1}-\frac{Df(x_{n-1})}{kT}\Delta t)^2}{4D\Delta t}} \\
&= (\frac{1}{\sqrt{4\pi D\Delta t}})^{N-1} \int \prod_{n=1}^{N-1} dx_n e^{-\frac{(x_n-x_{n-1}-\frac{Df(x_{n-1})}{kT}\Delta t)^2}{4D\Delta t}} \\
&\simeq (\frac{1}{\sqrt{4\pi D\Delta t}})^{N-1} \int \prod_{n=1}^{N-1} dx_n e^{-\sum_n \frac{\left((x_n-x_{n-1})/\Delta t-\frac{Df(x_{n-1})}{kT}\right)^2}{4D}\Delta t} \\
&\equiv \int Dx(t) e^{-\frac{1}{4D}\int_0^t dt(\dot{x}(t)-\frac{Df(x(t))}{kT})^2}
\end{aligned}$$

with the boundary conditions $x(t) = x_f$ and $x(0) = x_0$ and, as usual for path integrals, the infinite normalization constant $(\frac{1}{4\pi D\Delta t})^{N-1}$ (for $N \to \infty$) has been absorbed into the definition of $Dx(t)$.

Note that $\int dx_f P(x_f, t|x_0, 0) = 1$ as it should.

Chapter 2

First passage processes.

Many times, we are not interested in knowing the probability to be at a position x at time t but rater the probability for getting to position x at time t *for the first time*. This seemingly small difference in reality has dramatic consequences and is dealt within the framework of the *first passage* theory.

A simple example of a first passage process is the gambling discussed in the first lecture - when the gambler looses al his money, its an absorbing boundary, and the game ends. The question is in what time the gambler will reach this unfortunate state. Another classical example is the drunkard's walk that ends when the drunkard gets either to the gutter or a police station, which both serve as absorbing boundaries. The probability to get to either of the absorbing boundaries in time t is very different from the probability to reach them if they were just regular points, because it does not include all the trajectories that pass through the point before time t.

2.1 First example: Gambler's ruin problem.

The probability to loose all the money starting from n is described by the following equation:

$$P(n \to 0) = \frac{1}{2}P(n-1 \to 0) + \frac{1}{2}P(n+1 \to 0) \tag{2.1}$$

Looking for a solution in the form $P(n \to 0) = \lambda^n$, we get $(\lambda - 1)^2 = 0$ and therefore $\lambda = 1$. That is, the gambler is bound to loose all his money with probability one, no matter how much money he starts with.

On the other hand $\langle n \rangle(t) = n_0$ as can be shown using the forward Master equation in the definition of $\langle n \rangle$.

$$\dot{\langle n \rangle} = \sum_{n=1}^{\infty} n\dot{P}_n = 0 \tag{2.2}$$

In a more general case, of biased random walk with the absorbing boundary at $n = 0$, same reasoning gives

$$Pn \to 0 = qP(n-1 \to 0) + pP(n+1 \to 0) \tag{2.3}$$

Solving it again with $P_n = \lambda^n$ gives an equation for λ:

$$p\lambda^2 - \lambda + q = 0$$

which has two solutions: $\lambda = 1$ and $\lambda = q/p$. The general solution is $P_n = A + B(q/p)^n$ with the boundary conditions $P_0 = 1$ and $P_L = 0$. Finally

$$P_n = \frac{(q/p)^L - (q/p)^n)}{(q/p)^L - 1}$$

, which has two different limits when $L \to \infty$: $P_n \to 1$ for $q > p$ and $P_n \to (q/p)^n$ for $q < p$. Note that for the unbiased random walk, $p = q$, $P_n = 1$ as we already know.

Another way to see this is use the recursion, which gives

$$P_n = nP_1 - (n-1)p_0$$

. After using boundary condition $P_L = 0$, we get $P_n = 1 - n/L$, same as the exact results in the limit $L \to \infty$.

Time. If we are interested in the *overall* time to *either* be absorbed at zero, or to disappear to infinity, it is described by the familiar backward equation:

$$T_n = \tau + qT_{n-1} + pT_{n+1} \tag{2.4}$$

with the boundary conditions $T_0 = 0$ and $T_L = 0$. where $\epsilon = p - q$ and $p > q$. We use the usual trick of assuming an absorbing boundary condition at $n = L$ and letting $L \to \infty$.

We look for a solution in the form $T_n = A - \tau n/\epsilon + C(q/p)^n$. From the boundary conditions $T_0 = 0$ and $T_L = 0$, $C = -A$; $A = \frac{\tau L}{\epsilon}\frac{1}{(q/p)^L - 1}$ and finally

$$T_n = \frac{\tau L}{\epsilon}(-n/L + \frac{(q/p)^n - 1}{(q/p)^L - 1})$$

In the limit $L \to \infty$, $T_n \to \infty$ for $q/p < 1$ and $T_n \to \frac{\tau n}{|\epsilon|}$ for $q/p > 1$.

2.1.1 Derivation of the equation for the mean of the biased random walk

The (forward) Master equation in this case is

$$\begin{aligned} \dot{P}_0 &= r_{\leftarrow} P_1 \\ \dot{P}_1 &= -rP_1 + r_{\leftarrow} P_2 \\ \dot{P}_n &= r_{\rightarrow} P_{n-1} + r_{\leftarrow} P_{n+1} - rP_n \end{aligned} \tag{2.5}$$

where $r = r_{\rightarrow} + r_{\leftarrow}$.

Thus (re-indexing the sums, $m = n + 1$ etc)

$$\begin{aligned} \frac{d}{dt}\langle n \rangle &= \sum_{n=0}^{\infty} n\dot{P}_n = -rP_1 + r_{\leftarrow}P_2 + r_{\rightarrow}\sum_{n=1}^{\infty}(-rP_n + r_{\rightarrow}P_{n-1} + r_{\leftarrow}P_{n+1}) \\ &= -rP_1 + r_{\leftarrow}P_2 + r_{\rightarrow}\sum_{m=1}^{\infty}(m+1)P_m + r_{\leftarrow}\sum_{p=3}^{\infty}(p-1)P_p - r\sum_{n=2}^{\infty}P_n \\ &= -rP_1 + r_{\leftarrow}P_2 + r_{\rightarrow}\sum_{m=1}^{\infty}mP_m + r_{\leftarrow}\sum_{p=3}^{\infty}pP_p - r\sum_{n=2}^{\infty}P_n + r_{\rightarrow}\sum_{m=1}^{\infty}P_m - r_{\leftarrow}\sum_{p=3}^{\infty}pP_n \\ &= -rP_1 + r_{\leftarrow}P_2 + r_{\rightarrow}\sum_{m=1}^{\infty}mP_m + r_{\leftarrow}(\sum_{p=1}^{\infty}pP_p - P_1 - 2P_2) - r(\sum_{n=1}^{\infty}nP_n - P_1) \\ &+ r_{\rightarrow}(1 - P_0) - r_{\leftarrow}(1 - P_1 - P_2 - P_3) = (1 - P_0(t))(r_{\rightarrow} - r_{\leftarrow}). \end{aligned} \tag{2.6}$$

For a symmetric random walk its zero.

2.2 Another example: continuous limit of a random walk.

Let us consider a simple example of a random walk with an absorbing boundary condition at either both 0 and L or a reflective boundary condition at 0 and absorbing at L.

Following the arguments presented in class, the probability to get to, say, 0 starting from x_0 in *any time* is described by the following equation:

$$P(x_0 \to 0) = p(x_0)P(x_0 + a \to 0) + q(x_0)P(x_0 - a \to 0) \tag{2.7}$$

Expanding to the second order in a, we get:

$$(p(x_0) - q(x_0))a\frac{\partial}{\partial x_0}P(x_0) + \frac{1}{2}a^2\frac{\partial^2}{\partial x_0^2}P(x_0) = 0 \tag{2.8}$$

The boundary conditions are $P(0) = P(L) = 0$ for absorbing boundary conditions. For a reflective boundary condition, $P(0) = P(a)$ and $\frac{\partial P(x_0)}{\partial x_0} = 0$.

Similarly, for $T(x_0)$,

$$T(x_0 \to 0) = \tau + p(x_0)T(x_0 + a \to 0) + q(x_0)T(x_0 - a \to 0) \tag{2.9}$$

so that

$$(p(x_0) - q(x_0))a\frac{\partial}{\partial x_0}P(x_0) + \frac{1}{2}a^2\frac{\partial^2}{\partial x_0^2}P(x_0) = -\tau \tag{2.10}$$

with the boundary conditions $T(x_0) = 0$ at an absorbing boundary and $\frac{\partial T(x_0)}{\partial x_0} = 0$ at a reflective boundary.

Let us define the operator $\pounds_{x_0} \equiv (p(x_0) - q(x_0))\frac{a}{\tau}\frac{\partial}{\partial x_0} + D\frac{\partial^2}{\partial x_0^2}$. Then the above is compactly written as

$$\pounds_{x_0}P(x_0) = 0$$

and

$$\pounds_{x_0}T(x_0) = -1$$

.

We could also define the discrete operator

$$\hat{M}_b F) \equiv \frac{1}{\tau}(p(x_0)F(x_0 + a)0) + q(x_0)F(x_0 - a) - F(x_0)$$

. In the matrix form, the operator $\hat{M}_b = \hat{M}_f^T$ is the transpose of forward Master operator

2.3 Backward Master and Fokker-Planck equation

These were heuristic arguments. Here we put them on a solid mathematical basis. The developed mathematical framework will also serve us later for more complication cases , where heuristics gets shaky.

In the previous chapter, we derived the Master and the Fokker-Planck equations for the probability $P(x,t)$ starting at x_0 at time $t_0 = 0$. Including now the initial conditions explicitly, we can have another look on the $P(x,t|x_0,0)$ using the arguments similar to those of the preceding section.

$$P(x,t+\tau|x_0,0) = p(x_0 \to x_0+a,\tau)P(x,t+\tau|x_0+a,\tau) + p(x_0 \to x_0-a,\tau)P(x,t+\tau|x_0-a,\tau)$$
$$= p(x_0)P(x,t|x_0+a,0) + q(x_0)P(x,t|x_0-a,0)$$

where we have used the *stationarity*: $P(y,t_1|z,t_2) = P(y,t_1-t_2|z,0)$. Its not a very onerous condition; the Markov processes with transition rates without explicit dependence on time almost always satisfy it. For instance, the standard Gaussian solution for the random walk definitely satisfies it, because it depends only on the elapsed time $t-t_0$ and not independently on t and t_0.

Expanding in τ, we get

$$\dot{P}(x,t|x_0,0) = \frac{1}{\tau}(p(x_0)P(x,t|x_0+a,0) + q(x_0)P(x,t|x_0-a,0) - P(x,t|x_0,0)) \tag{2.11}$$

Similarly to the forward Master equation, the Backward equation can be written in the matrix form

$$\dot{\vec{P}}(t) = \hat{M}_b \cdot \vec{P}(t)$$

where $\vec{P}_i = P(x,t|x_i,0)$ and $\hat{M}_b$ is defined by the equation 2.3. Note that $\hat{M}_b$ is the transpose of the $\hat{M}_f$.

Written in terms of transition rates of the transition matrix the backward equation can be written as

$$\dot{P}_{ij} = r_{j+1,j}P_{i,j+1} + r_{j,j-1}P_{i,j-1} - P_{ij} \tag{2.12}$$

where P is a *tensor* whose components are the conditional probabilities $\hat{P}_{ij} = P(x_i,t|x_j,0)$.

Upon examination, it is clear that it is a transpose of the forward equation

$$\dot{P}_{ij} = r_{i,i+1}P_{i-1,j} + r_{i,j+1}P_{i+1,j} - P_{ij} \tag{2.13}$$

Thus, the most general formulation of the Master equation that subsumes both the forward and the backward equations is

$$\frac{d}{dt}\hat{P} = \hat{M} \cdot \hat{P} \tag{2.14}$$

Backward Fokker-Planck equation.

Expanding $P(x,t|x_0 \pm a,0) \simeq P(x,t|x_0,0) \pm a\frac{\partial}{\partial x_0}P(x,t|x_0,0) + \frac{1}{2}a^2\frac{\partial^2}{\partial x_0^2}P(x,t|x_0,0)$ we get:

$$\frac{\partial}{\partial t}P(x,t|x_0,0) = (p(x_0)-q(x_0))a/\tau\frac{\partial}{\partial x_0}P(x,t|x_0,0) + \frac{1}{2}a^2/\tau\frac{\partial^2}{\partial x_0^2}P(x,t|x_0,0) \equiv \pounds_{x_0}P(x,t|x_0,0) \tag{2.15}$$

If we want to connect it to the potential landscape, we remember that $(p(x_0)-q(x_0))a/\tau = f(x_0)D/(k_BT)$, where $f(x)$ is the force at a position x.

2.3.1 Survival probability

In a similar spirit, the probability that the walker is *still* in the interval at time t if it started at x_0 at time $t_0 = 0$ is

$$S(t|x_0) = \int_a^b dx P(x,t|x_0,0)$$

$S(t)$ satisfies the following equation (using the backward Fokker-Planck equation):

$$\frac{\partial}{\partial t}S(t|x_0) = \int_0^L dx \pounds_{x_0} P(x,t|x_0,0) = \pounds_{x_0} S(t|x_0) \tag{2.16}$$

On the other hand, using the forward Fokker-Planck equation

$$\frac{\partial}{\partial t}S(t|x_0) = -\int_0^L dx \frac{\partial J(P(x,t|x_0,0))}{\partial x} = J(0,t) - J(L,t) \equiv -R(t) \tag{2.17}$$

which simply means that the probability to be in the interval decreases through the flux at the boundaries. In heuristic terms - random walkers flow out of the interval through the boundaries.

Therefore, using the fact that $S(0|x_0) = 1$,

$$S(t|x_0) = 1 - \int_0^t R(t')dt'$$

where $R(t) = -(J(0,t) - J(L,t))$. However, essentially dy definition, $R(t)$ is the probability density of the exit times for a walker that starts at x_0 at time $t_0 = 0$, because $S(t|x_0)$ is the cumulative for the exit process.

The mean time in the interval is

$$T(x_0) \equiv \langle t \rangle_{x_0} = \int_0^\infty dt' R(t') t' = \int_0^\infty dt' S(t'|x_0) \tag{2.18}$$

Thus

$$\pounds_{x_0} \langle t \rangle_{x_0} = \int_0^\infty dt' \pounds_{x_0} S(t'|x_0) = \int_0^\infty dt' \frac{\partial}{\partial t} S(t|x_0) = S(\infty|x_0) - S(0|x_0) = -1$$

where we have used integration by parts and assumed that everything vanishes at infinity. QED.

Derivation with the backward Master equation. See class notes.

2.4 Directional probabilities and times

Similarly, one might ask the question - what are the *directional* times to be absorbed at either of the boundaries.

To this end, the probability to leave the interval by time t, $1 - S(t)$, can be explicitly separated into the probability to leave through the left side and the right side, respectively:

$$1 - S(t|x_0) = Q_\rightarrow(t|x_0) + Q_\leftarrow(t|x_0) \tag{2.19}$$

where, according to the above discussion,

$$Q_\leftarrow(t|x_0) = \int_0^t dt' J(0,t')$$
$$Q_\rightarrow(t|x_0) = \int_0^t dt' J(L,t')$$

The total probabilities to exit to the right or left are then $P_\leftarrow = Q_\leftarrow(\infty|x_0)$ and $P_\rightarrow = Q_\rightarrow(\infty|x_0)$ With this normalization, the *probability density* of the distribution of the exit times to the left is $J(0,t)/P_\leftarrow$ and to the right is $J(L,t)/P_\rightarrow$.

Auxiliary Lemma. The flux $J(x,t|x_0)$ satisfies the backward Fokker-Planck/Master equation. *Proof:*

$$\frac{\partial}{\partial t}J(x,t|x_0) = (p(x)-q(x))\frac{a}{\tau}\frac{\partial}{\partial t}P(x,t|x_0) - D\frac{\partial^2}{\partial x^2}\frac{\partial}{\partial t}P(x,t|x_0)$$
$$= (p(x)-q(x))\frac{a}{\tau}\pounds_{x_0}P(x,t|x_0) - D\frac{\partial^2}{\partial x^2}\pounds_{x_0}P(x,t|x_0) = \pounds_{x_0}J(x,t|x_0) \tag{2.20}$$

Now, the average time to exit to the right is $T_{\rightarrow}(x_0)\int_0^t dt' t' J(L,t'|x_0)/P_{\rightarrow}$. Thus

$$\pounds_{x_0}P_{\rightarrow}(x_0)T_{\rightarrow}(x_0) = \int_0^t dt' t' \pounds_{x_0}J(L,t'|x_0)$$
$$= \int_0^t dt' t' \frac{\partial}{\partial t'}J(L,t'|x_0) = -\int_0^t dt' J(L,t'|x_0) = -P_{\rightarrow}(x_0) \tag{2.21}$$

Similarly, for $P_{\rightarrow}(x_0)$ itself:

$$\pounds_{x_0}P_{\rightarrow}(x_0) = \int_0^t dt' \pounds_{x_0}J(L,t'|x_0) = \int_0^t dt' \frac{\partial}{\partial t'}J(L,t'|x_0) = J(L,\infty|x_0) - J(L,0|x_0) = 0 \tag{2.22}$$

because the flux through the right boundary is zero both at time $t=0$ and $t=\infty$.

2.4.1 Absorbtion probabilities and times through Master equation

Examples

Example 1: Calculate the mean first passage time (MFPT) for a particle staring at $0 < x < L$ with two absorbing boundaries ath $x = 0$ and $x = L$ escape through the right absorbing boundary

Solution. The probability to escape through the right ed is$p_{\rightarrow}(x) = x/L$. The MFPT is then described by the following ODE:

$$D\frac{d^2 p_{\rightarrow}(x)T_{\rightarrow}(x)}{dx^2} = -x/L \tag{2.23}$$

with the boundary conditions $Z(x) \equiv p_{\rightarrow}(x)T_{\rightarrow}(x) = 0$ both at $x=0$ and $x=L$.

Thus,

$$Z(x) = -\frac{x^3}{6DL} + Ax + B$$

From the boundary conditions $B=0$ and $A = L/(6D)$, so that

$$Z(X) = (L^2 - x^2)x/(6DL) \Rightarrow T_{\rightarrow} = LZ(x)/x = (L^2-x^2)/(6D)$$

which is similar to the expression with the reflective boundary at $x=0$ (derived in class). Not surprisingly, it diverges when $L \to \infty$.

The time to escape from the left boundary is more interesting:

$$D\frac{d^2 p_{\leftarrow}(x)T_{\leftarrow}(x)}{dx^2} = -1 + x/L$$

resulting in

$$T_{\leftarrow} = x(2L-x)/(6D)$$

which *also* diverges when $L \to \infty$. This is an unexpected result, which means that although in most realizations of the random walk, the walker returns to $x = 0$ in a finite time, some of the walkers that eventually end up at $x = 0$, spend a very long (diverging with L) time wandering within the interval.

Example 2: Kramers' problem Kramers' was the first to calculate the escape time from a potential well, as a model for the rates of chemical reactions.

Problem: calculate the MFPT from x_0 to x_1 (See Fig. 1)

Solution The backward Fokker Planck equation for $T(x)$ is

$$D\frac{d^2}{dx^2}T(x) + f(x)\frac{D}{k_BT}\frac{d}{dx}T(x) = -1 \tag{2.24}$$

with $f(x) = -dU(x)/dx$ and the boundary conditions $T(x_1) = 0$ and $dT(x_0)/dx = 0$. The latter can be understood noting that at a reflective boundary $T(0) = \tau + T(a) \Rightarrow dT(0)/dx = -\tau/a$ which tends to zero as a because we keep $D = a^2/(2\tau)$ constant as a and τ approach zero.

Denoting $R(x) = dT(x)/dx$ and looking for a solution in the form $R(x) = A(x)e^{U(x)/k_BT}$, we get

$$R(x) = (C - \frac{1}{D}\int_{x_0}^{x} dx' e^{-U(x')/k_BT})e^{U(x)/k_BT} \tag{2.25}$$

From the boundary condition at $x = x_0$, $C = 0$. Thus,

$$T(x) = C_1 - \frac{1}{D}\int_{x_0}^{x} dx' e^{U(x')/k_BT}\int_{x_0}^{x'} dx'' e^{-U(x'')/k_BT} \tag{2.26}$$

From the boundary condition $T(x_1) = 0$,

$$C_1 = \frac{1}{D}\int_{x_0}^{x_1} dx' e^{U(x')/k_BT}\int_{x_0}^{x'} dx'' e^{-U(x'')/k_BT}$$

and therefore

$$T(x_0) = C_1 = \frac{1}{D}\int_{x_0}^{x_1} dx' e^{U(x')/k_BT}\int_{x_0}^{x'} dx'' e^{-U(x'')/k_BT}$$

Its impossible to calculate this double integral for a general potential $U(x)$, but one can make use of a WKB-type approximation. Note that the main contribution to the second integral comes from the vicinity of x_0, and the main contribution to the first one comes from around $x = x_1$. Thus, we can expand around those:

$$\begin{aligned} T(x_0) &\simeq \frac{1}{D}\int_{x_0}^{x_1} dx e^{U_1/(k_BT) - \alpha/(k_BT)(x-x_1)^2/2)}\int_{x_0}^{x} dy e^{-U_0/(k_BT) - \beta/(k_BT)(x-x_0)^2/2)} \\ &\simeq \frac{1}{D}e^{(U_1-U_0)/(k_BT)}\int_{-\infty}^{\infty} dx e^{-\alpha(x-x_1)^2/2)}\int_{-\infty}^{\infty} dy e^{-\alpha(y-x_1)^2/2)} \simeq \frac{1}{D}e^{U_1-U_0}\frac{k_BT}{\sqrt{\alpha\beta}} \end{aligned} \tag{2.27}$$

Example : Absorbtion in 3D. Same arguments work in higher dimensions. *Question: particle starts at a position $a < r < b$ between two absorbing spheres at $r = a$ and $r = b$. What are the absorbtion probabilities and times?*

Probability. Probability to get absorbed at $r = a$ is given by the equation

$$\nabla^2 P(r) = 0 \;\Rightarrow\; \frac{1}{r^2}\frac{d}{dr}(r^2\frac{dP(r)}{dr}) = 0 \tag{2.28}$$

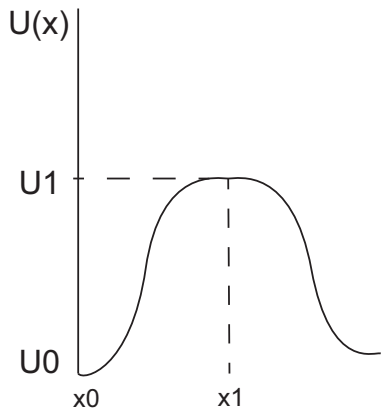

Figure 2.1: **Kramers potential**

with the boundary conditions $P(a) = 1$ and $P(b) = 0$. Thus

$$P(r) = B - A/r = \frac{a}{r}\frac{r-b}{a-b}$$

Note that $P(r) \to a/r$ when $b \to \infty$: unlike in 1D case, where it tends to 1. Also,$P(r) \to 0$ when $a \to 0$: the probability to get absorbed into a point is zero in 3D.

Time. Similarly the time to be absorbed at *either* of the boundaries, is

$$D\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dT(r)}{dr}) = -1 \tag{2.29}$$

with the boundary conditions $T(a) = T(b) = 0$. Thusly,

$$\begin{aligned} T(r) &= -A/r - r^2/(6D) + B = \frac{a^2}{6D}\left[1 + (a/b)^2 + b/a - (r/a)^2 - (b/r)(1 + b/a)\right] \\ &= \frac{(b-a)(r-a)(1+(a+b)/r)}{D} \end{aligned} \tag{2.30}$$

Example : Moran/Fisher-Wright model In the MFW model, a population of N individuals (fraction f of which are red and $1 - f$ are green) is updated by randomly choosing one to divide, and another one to die. So, at each time step, the fraction of the reds changes by

$$\begin{aligned} 1/N &\text{ with probability } f(1-f) \\ -1/N &\text{ with probability } f(1-f) \\ 0 &\text{ with probability } f^2 + (1-f)^2 \end{aligned}$$

The Backward equation for the probability of red fixation is:

$$P(f) = \frac{1}{2}P(f - 1/N) + \frac{1}{2}P(f + 1/N) \tag{2.31}$$

, which has solution $P = f$, as a simple substitution can prove. This is not surprising because its the same backward equation as for a simple symmetric random walk.

The time to fixation at either end is given by the equation

$$T(f) = \tau + (f^2 + (1-f)^2)T(f) + f(1-f)T(f - 1/N) + f(1-f)T(1 + 1/N) \tag{2.32}$$

Performing the Fokker-Planck expansion:

$$\frac{f(1-f)}{N^2}\frac{\partial^2 T(f)}{\partial^2} = -\tau \tag{2.33}$$

with the boundary conditions $T(0) = T(1) = 0$. Performing the two integrations, we get

$$T(f) = -\tau N^2[f\ln(f) + (1-f)\ln(1-f)]$$

Analogously, the *directional time* $T_r(f)$ for the fixation of reds can be obtained from the equation

$$Z(f) = \tau f + (f^2 + (1-f)^2)Z(f) + f(1-f)Z(f-1/N) + f(1-f)Z(1+1/N) \tag{2.34}$$

where $Z(f) = fT_r(f)$ with b.c's $Z(0) = Z(1) = 0$. Solving it gives

$$T_r(f) = \tau N^2(1-f)\ln(1-f)/f$$

Chapter 3

Population processes.

3.1 Birth-death processes.

3.1.1 Pure birth process

Let us consider a population of proliferating cells that divide with an average rate β, that is a cell has a chance βdt to produce off-spring in the timer interval dt. We shall denote the number of cells at time t as $n(t)$. For simplicity, we assume that at time $t = 0$, the population starts with a single progenitor cell. Thus, the *mean* population size at time t is $2^{\beta t}$. However, due to the inherent stochasticity of the division times, in different experiments, the actual number of cells at time t will be different. We now compute the *probability* of the population to grow to size n at time t. This probability $P_n(t)$ is described by the following equations []([see also Appendix for the derivation).

$$\begin{aligned} \dot{P}_1 &= -\beta P_1(t) \quad \text{for} \quad n = 1 \\ \dot{P}_n &= -\beta n P_n(t) + \beta(n-1)P_{n-1}(t) \quad \text{for} \quad n > 1 \end{aligned} \tag{3.1}$$

The equation for the mean population size $\langle n \rangle(t)$ is

$$\begin{aligned} \dot{\langle n \rangle}(t) = \beta \sum_{n=1}^{\infty} n \dot{P}_n(t) = \beta \sum_{n=2}^{\infty} \left(n(n-1)P_{n-1} - n^2 P_n \right) - \beta P_1 = \\ = \beta \sum_{m=1}^{\infty} \left((m+1)mP_m - \sum_{n=1}^{\infty} n^2 P_n \right) = -\sum_{m=1}^{\infty} mP_m = -\beta \langle n \rangle \end{aligned} \tag{3.2}$$

so that $\langle n(t) \rangle = e^{\beta t}$ grows exponentially, as expected.

The equations 3.1 can be solved iteratively:

$$\begin{aligned} P_1(t) &= e^{-\beta t} \quad \text{for} \;\; n = 1 \\ P_n(t) &= \beta(n-1)e^{-n\beta t} \int_0^t dt' e^{n\beta t'} P_{n-1}(t') \quad \text{for} \;\; n > 1 \end{aligned} \tag{3.3}$$

which leads to the general expression:

$$P_n(t) = e^{-n\beta t} \left(e^{\beta t} - 1 \right)^{n-1} = \frac{1}{\langle n(t) \rangle} \left(1 - \frac{1}{\langle n(t) \rangle} \right)^{n-1} \tag{3.4}$$

3.1.2 Pure death process.

Let us now consider an opposite process. A population of cells, starting with N individuals. The cells die with an average rate μ. Again, we ask what is the probability distribution of the number of surviving cells at time t, $P_n(t)$:

$$\frac{\partial P_n(t)}{\partial t} = \mu\left((n+1)P_{n+1} - nP_n\right) \tag{3.5}$$

With the equations for $n = N$ and $n = 0$:

$$\frac{\partial P_N(t)}{\partial t} = -\mu N P_N \quad \text{and} \quad \frac{\partial P_0(t)}{\partial t} = \mu P_1 \tag{3.6}$$

The equation for the mean $\langle n\rangle = \sum_{n=0}^{N} nP_n$ is

$$\dot{\langle n\rangle}(t) = \mu\sum_{n=0}^{N-1}\left(n(n+1)P_{n+1} - n^2P_n\right) - \mu N P_N = -\mu\sum_{n=0}^{N} nP_n \tag{3.7}$$

so that the *mean* population size $\langle n(t)\rangle = Ne^{-\mu t}$ decays exponentially.

As above, the equations () can be integrated iteratively, which gives for $P_{N-1} = Ne^{-\mu(N-1)t}(1-e^{-\mu t})$ and in general:

$$P_n(t) = \frac{N!}{n!(N-n)!}e^{-\mu nt}\left(1-e^{-\mu t}\right)^{N-n} \tag{3.8}$$

Interestingly, unlike a pure birth process, it is not an exponential distribution but a binomial distribution around the average $Ne^{-\mu t}$.

3.1.3 Full birth-death process

In this section we derive the probability distribution function for the full birth-death process, which is described by the following master equations:

$$\frac{\partial}{\partial t}P_n(t) = \beta(n-1)P_{n-1}(t) + \mu(n+1)P_{n+1}(t) - (\beta+\mu)nP_n(t) \tag{3.9}$$

with the boundary condition $\frac{\partial}{\partial t}P_0(t) = \mu P_1(t)$, and the initial condition $P_n(0) = \delta_{n,N}$.

Defining the generating function $G(z,t) = \sum_{n=0}^{\infty} z^n P_n(t)$ equation 3.9 becomes

$$\frac{\partial}{\partial t}G(z,t) = (\beta z^2 - (\beta+\mu)z + \mu)\frac{\partial}{\partial z}G(z,t) \tag{3.10}$$

with the initial condition $G(z,0) = z^N$ and boundary conditions $G(0,t) = 0$ and $G(1,t) = 1$.

Using the method of characteristics, we get

$$\frac{dt}{dr} = 1 \quad \frac{dz}{dr} = -(\beta z^2 - (\beta+\mu)z + \mu) \tag{3.11}$$

Thus,

$$z_0 = \frac{\mu - e^{-(\beta-\mu)r}(\beta z-\mu)/(z-1))}{\beta - e^{-(\beta-\mu)r}(\beta z-\mu)/(z-1)} \tag{3.12}$$

Now, $G(z,t) = F(z_0)$ such that for $z_0 > 0$ it satisfies the initial condition $G(z,0) = z^N$ and for $z_0 < 0$ satisfies the boundary condition $G(1,t) = 1$. The solution satisfying these conditions is:

$$G_N(z,t) = z_0^N = (\frac{(\mu\langle n(t)\rangle - \beta)z + \mu(1 - \langle n(t)\rangle)}{\beta(\langle n(t)\rangle - 1)z + \mu - \beta\langle n(t)\rangle})^N \tag{3.13}$$

where $\langle n(t)\rangle = e^{(\beta-\mu)t}$. It is interesting to note that the generating function $G_N(z,t) = G_1(z,t)^N$ and therefore the distribution function $P_n(t)$ is the sum of the distribution functions of the variables whose generating function is $G_1(z,t)$. Expanding $G_1(z,t)$ in Taylor series, we get:

$$\begin{aligned} P_n^1(t) &= \frac{(\langle n(t)\rangle - 1)^{n-1}\langle n(t)\rangle\beta^{n-1}(\beta-\mu)^2}{(\beta\langle n(t)\rangle - \mu)^{n+1}} \quad \text{for} n > 1 \\ P_0^1(t) &= \frac{\mu(\langle n(t)\rangle - 1)}{\beta\langle n(t)\rangle - \mu} \end{aligned} \tag{3.14}$$

3.2 Extinction probabilities and times

3.2.1 Extinction probability

In this section we calculate the probability that by the time t, the population is not extinct. For this we make two important notions: the probability flux to the extinct state $n = 0$ is $J(t) = \mu P_1(t)$. And therefore, the *extinction probability* by time t is $P_{\text{ext}}(t) = \int_0^t J(t')dt'$. From the equation 3.13:

$$P_1^N = \frac{\partial}{\partial z}G_N(z,t) = \frac{N(\mu e^{(\beta-\mu)t} - 1)^{N-1}e^{(\beta-\mu)t}(\beta-\mu)^2}{(\beta e^{(\beta-\mu)t} - \mu)^{N+1}} \tag{3.15}$$

and the probability to be extinct by the time t is

$$P_{\text{ext}}(t) = \mu\int_0^t P_1^N(t')dt' = \left(\frac{\mu e^{(\beta-\mu)t} - \mu}{\beta e^{(\beta-\mu)t} - \mu}\right)^N \tag{3.16}$$

Equation 3.16 is the main result of this section. It follows that for $\beta < \mu$, when the population is on average is exponentially contracting, the extinction probability

$$P_{\text{ext}} = \lim_{t\to\infty} P_{\text{ext}}(t) = 1 \tag{3.17}$$

is equal one - perhaps not surprisingly, the population becomes extinct with certainty.

In the case $\beta \geq \mu$, when the population is exponentially expanding *on average*, there is still a finite probability of extinction:

$$P_{\text{ext}} = \lim_{t\to\infty} P_{\text{ext}}(t) = \left(\frac{\mu}{\beta}\right)^N \tag{3.18}$$

It is interesting that this holds even for $\beta = \mu$, in which case the population becomes extinct with probability one, in finite time! In this marginal case,

$$P_{\text{ext}}(t) = \left(\frac{\mu t}{1+\beta t}\right)^N \tag{3.19}$$

3.2.2 Extinction times

The normalized (conditional) probability density of the distribution of the extinction time is $J(t)/P_{\text{ext}}$ and the mean extinction time is

$$\begin{aligned} T_N \equiv \langle t \rangle &= \int_0^\infty dt' t' J(t')/P_{\text{ext}} = \\ &= \int_0^\infty dt' t' \mu P_1^N(t')/P_{\text{ext}} = \int_0^\infty dt' t' \frac{\partial P_{\text{ext}}(t')}{\partial t'}/P_{\text{ext}} = \\ &= tP_{\text{ext}}(t)_0^\infty/P_{\text{ext}} - \int_0^\infty dt' P_{\text{ext}}(t')/P_{\text{ext}} = \int_0^\infty dt'(1 - P_{\text{ext}}(t'))/P_{\text{ext}} \end{aligned} \tag{3.20}$$

N=1 For $\mu > \beta$, the extinction time is then

$$T = -\frac{1}{\beta}\ln(1 - \beta/\mu)$$

and for $\mu < \beta$

$$T = -\frac{1}{\beta}\ln(1 - \mu/\beta)$$

3.2.3 Backward Fokker-Planck calculation of the extinction probabilities and times.

We could perform the same calculations using the backward Fokker-Planck formalism:

Probability

$$P_N = \frac{\beta}{\beta+\mu}P_{N+1} + \frac{\mu}{\beta+\mu}P_{N-1} \tag{3.21}$$

Seeking for a solution in a form $P_N = x^N$, we get for x:

$$x^N = px^{N+1} + qx^{N-1} \quad \Rightarrow \quad px^2 - x + q = 0 \tag{3.22}$$

where $p = \frac{\beta}{\beta+\mu}$ and $q = \frac{\mu}{\beta+\mu}$. Thus

$$x = \frac{1 \pm \sqrt{1-4pq}}{2p} = \frac{1 \pm \sqrt{1-(1-\epsilon^2)}}{1+\epsilon} = \frac{1 \pm \epsilon}{1+\epsilon}$$

From this, the general solution is $P_N = A + (q/p)^N$. We use the trick of a boundary condition at "infinity": $P_M = 0$ at some $M \to \infty$. That is, using the boundary conditions: $A+B = 1$ and $A+(q/p)^M = 0$. Thus,

$$\begin{aligned} P_N &= 1/(1-(p/q)^M) + (p/q)^M/(1-(p/q)^M)(q/p)^N \\ \text{taking } M &\to \infty \\ P_N &= 1 \text{ for } p < q \\ P_N &= (q/p)^N \text{ for } p > q \end{aligned}$$

Mean Extinction time

$$p_N T_N = \frac{1}{(\beta+\mu)N} + P_N + pP_{N+1} + qP_{N-1}T_{N-1} \tag{3.23}$$

Seeking again for a solution in the form $Z_N \equiv P_N T_N = \frac{1}{\beta+\mu}x^N$:**See homework.**

Chapter 4

Chemical reactions

Although often thought of in terms of average "law of mass action" kinetics, chemical reactions are inherently stochastic due to the random nature of the association and dissociation processes on the microscopic scale. At small numbers of reactant molecules - as often happens in cells - the stochastic fluctuations in the numbers of reactant molecules start to become important.

The important distinguishing feature of the chemical reactions is that the reaction rates typically depend on reactant concentrations and not their absolute numbers. Therefore, for large system volume V, there is a small parameter $1/V$ that allows systematic expansion of the chemical Master equation close to the deterministic average. Unlike the uncontrolled approximation of the Fokker-Planck equation, this is a rigorous approximation method, known as Van Kampen expansion.

4.1 Chemical Master equation

As an illustrative example, let us consider a simple reaction, where the molecules of reactant x are produced (or injected into the system) with a rate $\beta \equiv b_0 V$, and annihilate via binary collisions with each other at a rate μ (each binary collision removes two molecules). The deterministic equation for the average number of particles in the system $\langle n \rangle$ is

$$\frac{d}{dt}\langle n \rangle = \beta - 2\frac{1}{2}\mu\langle n \rangle \frac{\langle n \rangle}{V} \tag{4.1}$$

which translates into an equation for the density $\phi \equiv \langle n \rangle / V$:

$$\frac{d}{dt}\phi = \beta_0 - \mu\phi^2 \tag{4.2}$$

which is what is expected from naive chemical kinetics.

The Master equation for the number of molecules in the system, n, is

$$\dot{P}_n = \beta P_{n-1} - \mu\frac{n(n-1)}{2V}P_n + \mu\frac{(n+2)(n+1)}{2V}P_{n+2} - \beta P_n \ \text{ for } \ n > 0 \tag{4.3}$$

and $\dot{P}_0 = \mu P_2/V - \beta P_0$.

4.1.1 Deterministic (Law of Mass Action) limit of chemical kinetics

We can check if this Master equation reproduces the deterministic kinetics at large $n \gg 1$. After a sequence of manipulations, we get

$$\frac{d}{dt}\langle n\rangle = \sum_{n=1}^{\infty} n\dot{P}_n = ... = \beta - \frac{\mu}{V}\sum_{m=1}^{\infty} m(m-1)P_m = \beta - \frac{\mu}{V}(\langle n^2\rangle - \langle n\rangle)$$

For large n, one expects the law of large numbers to kick in (and it can be proven), so that $\frac{\langle n^2\rangle - \langle n\rangle^2}{\langle n\rangle} \simeq O(1)$ and thus $\langle n^2\rangle - \langle n\rangle \simeq \langle n\rangle^2$. This brings us back to the macroscopic deterministic equation (4.1).

4.1.2 Van Kampen expansion.

The expansion of the distribution of the reactant numbers around the deterministic thermodynamic limit can be made systematic.

First, we define the "raising" and "lowering" operators acting on P_n:

$$EP_n = P_{n+1} \quad \text{and} \quad E^{-1}P_n = P_{n-1} \tag{4.4}$$

Then the Master equation is compactly written as

$$\dot{P}_n = \beta_0 V(E^{-1} - 1)P_n + \frac{\mu}{2V}(E^2 - 1)((n(n-1)P_n)) \tag{4.5}$$

Now, remembering that n is a random variable, we make a variable change:

$$n = \langle n\rangle(t) + V^{1/2}\xi \tag{4.6}$$

where $\langle n\rangle(t)$ is the deterministic average, and ξ is a random variable that characterizes fluctuations around the mean. The first term is proportional to V because in chemical reactions the density $\phi = n/V$ is the intensive variable. All the fluctuations around the mean are subsumed in the second term, which is explicitly assumed to be proportional to $\sqrt{\langle n\rangle} \sim V^{1/2}$ based on the central limit theorem. The fluctuation in n by ± 1 correspond to a small fluctuation $\pm V^{-1/2}$ in the ξ.

The random variable ξ is then approximately continuous variable for $V \gg 1$ and the P_n can be rewritten as a new function $P_n(t) \to \Pi(\xi, t)$. The operator E can be expanded as follows:

$$E \simeq 1 + V^{-1/2}\frac{\partial}{\partial\xi} + V^{-1}\frac{\partial^2}{\partial\xi^2} + ... \tag{4.7}$$

because

$$EP_n = P_{n+1}(t) = \Pi(\xi + V^{-1/2}, t) = \Pi(\xi, t) + \sum_{k=0}^{...}(V^{-1/2})^k \frac{1}{k!}\frac{\partial^k}{\partial\xi^k}\Pi(\xi, t)$$

Accordingly,

$$E^{-1} \simeq 1 - V^{-1/2}\frac{\partial}{\partial\xi} + V^{-1}\frac{\partial^2}{\partial\xi^2} + ... \tag{4.8}$$

After substituting this into the Master equation, the left hand side transforms into

$$\frac{\partial}{\partial t}\Pi(\xi, t) = \frac{\partial}{\partial\xi}\Pi(\xi, t)\frac{d}{dt}\langle n\rangle(t)V^{-1/2} = \frac{\partial}{\partial\xi}\Pi(\xi, t)\frac{d\phi(t)}{dt})V^{1/2} \tag{4.9}$$

The right hand side transforms into

$$\begin{aligned} & \beta_0 V(-V^{-1/2}\frac{\partial}{\partial\xi} + \frac{1}{2}V^{-1}\frac{\partial^2}{\partial\xi^2}\Pi(\xi, t) \\ + \quad & \frac{1}{2}V^{-1}\mu\left[2V^{-1/2}\frac{\partial}{\partial\xi} + 2V^{-1}\frac{\partial^2}{\partial\xi^2}\right](V\phi + V^{1/2}\xi)(V\phi + V^{1/2}\xi - 1)\Pi(\xi, t) \end{aligned}$$

Collecting the corresponding terms in the powers of V, in the spirit of perturbation theory, we get at $V^{1/2}$:

$$\frac{d}{dt}\phi = \beta_0 + \mu\phi^2 \tag{4.10}$$

which is simply the deterministic limit kinetics, as it should.

To the next order (v^0), we get

$$\frac{\partial}{\partial t}\Pi(\xi,t)\frac{1}{2} = \beta_0(1+2\phi(t)^2)\frac{\partial^2}{\partial\xi^2}\Pi(\xi,t) + 2\mu\xi\phi(t)^2\frac{\partial}{\partial\xi}\Pi(\xi,t) \tag{4.11}$$

which is a more rigorous cousin of the Fokker-Planck equation.

At steady state, under a reasonable assumption that $\phi \ll 1$,

$$\frac{1}{2}\beta_0\frac{\partial}{\partial\xi}\Pi(\xi) = -2\mu\phi^2\Pi(\xi) \tag{4.12}$$

which gives, using $\phi^2 = \beta_0/\mu$ for the steady state concentration,

$$\Pi(\xi) \sim \exp(-4\xi^2\phi^2\mu/\beta_0) = \exp(-4\xi^2)$$

This confirms our intuition of Gaussian fluctuations around the steady state. In more complicated reactions, the fluctuations are not necessarily gaussian.