

Fokker-Planck Equation

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Fokker-Planck equation is a widely used equation that describes the time evolution of the probability of a distribution of Brownian particles that is subject to random forces. Such an equation can be derived in two steps:

1) Equation of motion for the probability density $\rho(x, v, t)$ to find the Brownian particle in an interval $(x, x + dx)$ and $(v, v + dv)$ at time t for one realization of the random force $\xi(t)$.

2) Average over many realizations of the random force to obtain the macroscopically observed probability density $P(x, v, t) = \langle \rho(x, v, t) \rangle_\xi$.

Consider the phase space (x, v) and the probability to find the particle in an interval $(x, x + dx)$ and $(v, v + dv)$ at time t is given $\rho(x, v, t)dx dv$. Since the total number of particles is conserved over the entire phase space

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dv \rho(x, v, t) = 1 \quad (1)$$

Now if we consider the rate of change of particles in volume V_0 of the phase space that has a surface S_0 , this rate of change is equal to the outflow of particles through the surface S_0 . Thus by continuity

$$\frac{\partial}{\partial t} \int_{V_0} dV \rho(x, v, t) = - \int_{S_0} d\vec{S} \cdot \dot{\vec{x}} \rho(x, v, t) \quad (2)$$

where $\dot{\vec{x}} = (\dot{x}, \dot{v})$ is the velocity in phase space [dot represents the time derivative]. This is simply the ‘‘Continuity Equation’’ in phase space. By Gauss’ Theorem

$$\int_{S_0} d\vec{S} \cdot \dot{\vec{x}} \rho(x, v, t) = \int_{V_0} dV \vec{\nabla} \cdot [\dot{\vec{x}} \rho(x, v, t)] \quad (3)$$

where $\vec{\nabla} = (\partial_x, \partial_v)$. Therefore

$$\frac{\partial}{\partial t} \rho(x, v, t) = - \frac{\partial}{\partial x} [\dot{x} \rho(x, v, t)] - \frac{\partial}{\partial v} [\dot{v} \rho(x, v, t)] \quad (4)$$

since we can arbitrarily choose the volume V_0 in the phase space.

For Brownian motion of a particle in a potential $V(x)$ providing force $F(x) = -\partial_x V(x)$,

$$\begin{aligned} \frac{dx}{dt} &= v \\ \frac{dv}{dt} &= -\gamma \frac{v}{m} + \frac{F(x)}{m} + \frac{\xi(t)}{m} \end{aligned} \quad (5)$$

therefore

$$\begin{aligned} \frac{\partial}{\partial t} \rho(x, v, t) &= - \frac{\partial}{\partial x} [\dot{x} \rho(x, v, t)] - \frac{\partial}{\partial v} [\dot{v} \rho(x, v, t)] \\ &= - \frac{\partial}{\partial x} [v \rho(x, v, t)] + \frac{\partial}{\partial v} \left[\gamma \frac{v}{m} \rho(x, v, t) \right] - \frac{\partial}{\partial v} \left[\frac{F(x)}{m} \rho(x, v, t) \right] - \frac{\partial}{\partial v} \left[\frac{\xi(t)}{m} \rho(x, v, t) \right] \\ &= -L_0 \rho(x, v, t) - L_1 \rho(x, v, t) \end{aligned} \quad (6)$$

where the operators L_0 and L_1 are

$$\begin{aligned} L_0 &= v \frac{\partial}{\partial x} - \frac{\gamma}{m} v - \frac{\gamma}{m} v \frac{\partial}{\partial v} + \frac{F(x)}{m} \frac{\partial}{\partial v} \\ L_1 &= \frac{\xi(t)}{m} \frac{\partial}{\partial v} \end{aligned} \quad (7)$$

To get to the observable probability density, we need to average over the various realizations of the random force $\xi(t)$

$$P(x, v, t) = \langle \rho(x, v, t) \rangle_\xi \quad (8)$$

To evaluate this average, define

$$\rho(x, v, t) = e^{-L_0 t} \sigma(x, v, t) \quad (9)$$

which implies

$$\frac{\partial}{\partial t} \sigma(x, v, t) = -e^{L_0 t} L_1 e^{-L_0 t} \sigma(x, v, t) \equiv -V(t) \sigma(x, v, t) \quad (10)$$

The formal solution to this equation is

$$\sigma(x, v, t) = \exp \left[- \int_0^t dt_1 V(t_1) \right] \sigma(x, v, 0) \quad (11)$$

Averaging over the random force realizations

$$\langle \sigma(x, v, t) \rangle_\xi = \langle \exp \left[- \int_0^t dt_1 V(t_1) \right] \rangle_\xi \sigma(x, v, 0) \quad (12)$$

which upon using the cumulant expansion relation

$$\langle e^{-i\Phi(t)} \rangle = \exp \left[\sum_{n=1}^{\infty} \frac{(-i)^n}{n!} c_n \right] \quad (13)$$

gives (assuming that the random force is Gaussian implying that only second cumulant is non-zero equivalent to stating that only even moments are non-zero)

$$\langle \sigma(x, v, t) \rangle_\xi = \exp \left[\frac{1}{2} \int_0^t dt_1 \int_0^t dt_2 \langle V(t_1) V(t_2) \rangle_\xi \right] \sigma(x, v, 0) \quad (14)$$

Thus we evaluate the average in the exponential

$$\begin{aligned} \frac{1}{2} \int_0^t dt_1 \int_0^t dt_2 \langle V(t_1) V(t_2) \rangle_\xi &= \frac{1}{2} \int_0^t dt_1 \int_0^t dt_2 \langle e^{L_0 t_1} \frac{\xi(t_1)}{m} \frac{\partial}{\partial v} e^{-L_0 t_1} e^{L_0 t_2} \frac{\xi(t_2)}{m} \frac{\partial}{\partial v} e^{-L_0 t_2} \rangle_\xi \\ &= \frac{1}{2} \int_0^t dt_1 \int_0^t dt_2 \frac{\langle \xi(t_1) \xi(t_2) \rangle_\xi}{m^2} e^{L_0 t_1} \frac{\partial}{\partial v} e^{-L_0 t_1} e^{L_0 t_2} \frac{\partial}{\partial v} e^{-L_0 t_2} \\ &= \frac{1}{2} \int_0^t dt_1 \int_0^t dt_2 \frac{g \delta(t_1 - t_2)}{m^2} e^{L_0 t_1} \frac{\partial}{\partial v} e^{-L_0 t_1} e^{L_0 t_2} \frac{\partial}{\partial v} e^{-L_0 t_2} \\ &= \frac{1}{2} \int_0^t dt_1 \frac{g}{m^2} e^{L_0 t_1} \frac{\partial^2}{\partial v^2} e^{-L_0 t_1} \end{aligned} \quad (15)$$

where we have used the Gaussian nature of the random force i.e. $\langle \xi(t_1) \xi(t_2) \rangle_\xi = g \delta(t_1 - t_2)$. Thus

$$\langle \sigma(x, v, t) \rangle_\xi = \exp \left[\frac{g}{2m^2} \int_0^t dt_1 e^{L_0 t_1} \frac{\partial^2}{\partial v^2} e^{-L_0 t_1} \right] \sigma(x, v, 0) \quad (16)$$

Taking the time-derivative of the above equation

$$\frac{\partial}{\partial t} \langle \sigma(x, v, t) \rangle_\xi = \frac{g}{2m^2} e^{L_0 t} \frac{\partial^2}{\partial v^2} e^{-L_0 t} \langle \sigma(x, v, t) \rangle_\xi \quad (17)$$

which translates to

$$\frac{\partial}{\partial t} \langle \rho(x, v, t) \rangle_\xi = -L_0 \langle \rho(x, v, t) \rangle_\xi + \frac{g}{2m^2} \frac{\partial^2}{\partial v^2} \langle \rho(x, v, t) \rangle_\xi \quad (18)$$

which is the Fokker-Planck equation in terms of the macroscopic probability density

$$\frac{\partial}{\partial t} P(x, v, t) = -v \frac{\partial}{\partial x} P(x, v, t) + \frac{\partial}{\partial v} \left[\left(\frac{\gamma}{m} v - \frac{F(x)}{m} \right) P(x, v, t) \right] + \frac{g}{2m^2} \frac{\partial^2}{\partial v^2} P(x, v, t) \quad (19)$$

In absence of an external force and in thermal equilibrium ($\partial_t P = 0$), the probability distribution is given by the Boltzmann factor

$$P_0 \propto e^{-\beta m v^2 / 2} \Rightarrow \partial_v P_0 = -\beta m v P_0 \quad (20)$$

Hence

$$\begin{aligned} 0 &= \frac{\partial}{\partial v} \left[\frac{\gamma}{m} v P_0(v) \right] + \frac{g}{2m^2} \frac{\partial^2}{\partial v^2} P_0(v) \\ 0 &= \frac{\partial}{\partial v} \left[\frac{\gamma}{m} v P_0(v) \right] - \frac{g}{2m^2} \frac{\partial}{\partial v} \beta m v P_0 \\ 0 &= \frac{\partial}{\partial v} \left[\left(\frac{\gamma}{m} - \frac{\beta g}{2m} \right) v P_0(v) \right] \end{aligned} \quad (21)$$

which implies

$$g = 2\gamma k_B T \quad (22)$$

MATHEMATICAL RELATIONS

Moments and Characteristic Function

Probability distribution functions (PDF) are normalized:

$$\int_{-\infty}^{\infty} dx P(x) = 1 \quad (23)$$

which implies that the Fourier component of PDF at $k = 0$ is unity. The Fourier transform of the PDF can be defined as

$$P(k) = \int_{-\infty}^{\infty} dx e^{-ikx} P(x) \quad (24)$$

and from the normalization condition $P(k = 0) = 1$. The function $P(k)$ is referred to as the ‘‘Characteristic Function’’. The moments of the PDF can be thereby expressed in terms of the derivatives of the Characteristic Function.

$$\begin{aligned} m_1 = \langle x \rangle &= \int_{-\infty}^{\infty} dx x P(x) = i \frac{\partial P(k)}{\partial k} \Big|_{k=0} \\ m_2 = \langle x^2 \rangle &= \int_{-\infty}^{\infty} dx x^2 P(x) = i^2 \frac{\partial^2 P(k)}{\partial k^2} \Big|_{k=0} \\ &\vdots \\ m_n = \langle x^n \rangle &= \int_{-\infty}^{\infty} dx x^n P(x) = i^n \frac{\partial^n P(k)}{\partial k^n} \Big|_{k=0} \end{aligned} \quad (25)$$

Therefore

$$P(k) = \sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} m_n \quad (26)$$

Cumulants and Cumulant Generating Function

From the relation between the PDF and the characteristic function

$$P(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} P(k) \quad (27)$$

a “Cumulant Generating Function” $\psi(k)$ is defined as

$$P(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} e^{\psi(k)} \quad (28)$$

where $\psi(k) = \text{Log}[P(k)]$ is the function whose Taylor series coefficients at the origin $k = 0$ are the “Cumulants”.

$$c_n = \left. \frac{1}{i^n} \frac{\partial^n \psi(k)}{\partial k^n} \right|_{k=0} \quad (29)$$

Therefore

$$\begin{aligned} \psi(k) &= -ikc_1 - \frac{1}{2!}k^2c_2 \dots \\ &= \sum_{n=1}^{\infty} \frac{(-ik)^n}{n!} c_n \end{aligned} \quad (30)$$

Comparing to the Characteristic function expansion in terms of moments

$$\psi(k) = \sum_{n=1}^{\infty} \frac{(-ik)^n}{n!} c_n = \text{Log} \left[\sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} m_n \right] \quad (31)$$

implies

- $c_1 = m_1$ which is the “Mean”
- $c_2 = m_2 - m_1^2 = \sigma^2$ which is the “Variance” [σ : Standard Deviation]
- $c_3 = m_3 - 3m_1m_2 + 2m_1^3$ which is the “Skewness”
- $c_4 = m_4 - 3m_2^2 - 4m_1m_3 + 12m_1^2m_2 - 6m_1^4$ which is the “Kurtosis”

Therefore

$$P(k) = \exp \left[\sum_{n=1}^{\infty} \frac{(-ik)^n}{n!} c_n \right] = \sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} m_n \quad (32)$$

which implies

$$P(k=1) = \exp \left[\sum_{n=1}^{\infty} \frac{(-i)^n}{n!} c_n \right] = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} m_n \quad (33)$$

Consider the following average

$$\begin{aligned} \langle e^{-i\Phi(t)} \rangle &= \left\langle \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \Phi(t)^n \right\rangle \\ &= \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \langle \Phi(t)^n \rangle \\ &= \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} m_n \\ &= \exp \left[\sum_{n=1}^{\infty} \frac{(-i)^n}{n!} c_n \right] \end{aligned} \quad (34)$$