Stochastic Equations and Processes in physics and biology

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Lecture 5:

Ito and Stratonovich calculus, the Fokker-Planck equation

Integration of stochastic equations

Kiyosi Itô (1915-2008) Japanese mathematician

Integration of stochastic equations

Ruslan Leont'evich Stratonovich (1930-1997) Russian mathematician

Multiplicative noise

General stochastic equation

$$\dot{x}(t) = f(x(t)) + g(x(t))\xi(t), \quad \xi(t)\ldots \text{white noise}$$

Formal solution

$$\begin{aligned} x(T) &= x(t_0) + \int_{t_0}^{T} \dot{x}\, dt = \int_{t_0}^{T} [f(x(t))dt + g(x(t))\xi(t)dt] \\ &= \int_{t_0}^{T} [f(x(t))dt + g(x(t))dw(t)] \end{aligned}$$

Stochastic itegration

For a Wiener process $x(t)$ consider the integral

$$\int_0^T x(t)dx(t)$$

Mean-square limit sense

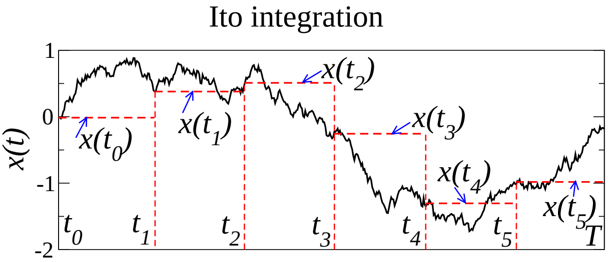
A sequence of random variables $X_n(\omega)$ converges to $X(\omega)$ in the sense of the mean-square limit, if

$$\lim_{n\to\infty} \int d\omega \, p(\omega)[X_n(\omega) - X(\omega)]^2 = 0$$

Ito interpretation

Riemann sum

$$I = \langle \lim_{N\to\infty} \sum_{i=0,N-1} x(t_i)[x(t_{i+1}) - x(t_i)] \rangle_{\mathrm{mean-square}}$$



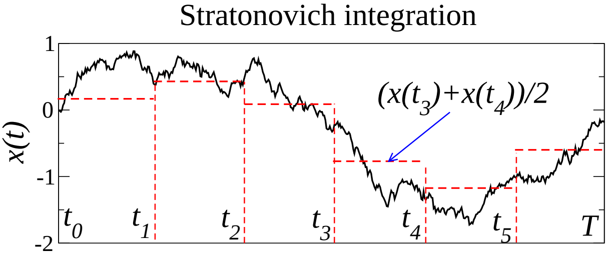
Mean-square limit of the Ito sum

$$I = \frac{1}{2}[x(T)^2 - x(t_0)^2] - \frac{T}{2}$$

Stratonovich interpretation

Riemann sum

$$S = \langle \lim_{N\to\infty} \sum_{i=0,N-1} \frac{1}{2}(x(t_i) + x(t_{i+1}))[x(t_{i+1}) - x(t_i)]\rangle_{\text{mean-square}}$$



Mean-square limit of the Stratonovich sum

$$S = \frac{1}{2}[x(T)^2 - x(t_0)^2]$$

Integration of Ito sde

Consider a general Ito stochastic equation

$$(I)\ dx = f(x)dt + g(x)dw(t), \quad (w(t) \ldots \text{ Wiener process})$$

Forward Euler's method

According to the definition of the Ito interpretation, the process $x_i = x(t_i)$ is generated by the forward Euler's method:

$$\begin{aligned} x_{i+1} &= x_i + \Delta t f(x_i) + g(x_i)\Delta w_i, \quad (i = 0, 1, 2, 3, \ldots) \\ \Delta w_i &= \sqrt{\Delta t} N(0, 1) \end{aligned}$$

Integration of Stratonovich sde

Consider a Stratonovich stochastic equation

$$(S)\ dx = g(x)dw(t), \quad (w(t) \ldots \text{ Wiener process})$$

For simplicity we set $f(x) = 0$
According to the definition of the Stratonovich interpretation

$$\begin{aligned} x_{i+1} &= x_i + g\left(\frac{x_{i+1} + x_i}{2}\right)\Delta w_i, \\ \Delta w_i &= N(0,1)\sqrt{\Delta t}. \end{aligned}$$

Implicit scheme

Note that this scheme is implicit, as one needs to solve for x_{i+1}

Integration of Stratonovich sde

Note that

$$\frac{x_{i+1} + x_i}{2} = x_i + \frac{x_{i+1} - x_i}{2}$$

Taylor expansion, assuming small $\Delta x = x_{i+1} - x_i$

$$x_{i+1} = x_i + \left[g(x_i) + g'(x_i) \frac{\Delta x}{2} \right] \Delta w_i$$

Solving for x_{i+1}

$$x_{i+1} = \left[x_i + g(x_i)\Delta w_i - g'(x_i)\frac{x_i}{2}\Delta w_i \right] \left(1 - \frac{g'(x_i)}{2}\Delta w_i \right)^{-1}$$

Integration of Stratonovich sde

To the order of Δt **and** $\Delta w_i \sim \sqrt{\Delta t}$

$$\begin{aligned} x_{i+1} &= \left[x_i + g(x_i)\Delta w_i - g'(x_i)\frac{x_i}{2}\Delta w_i\right]\left(1 + \frac{g'(x_i)}{2}\Delta w_i\right) \\ &= \left[x_i + g(x_i)\Delta w_i + \frac{1}{2}g(x_i)g'(x_i)(\Delta w_i)^2\right] + O(dt\,\Delta w_i). \end{aligned}$$

Because $\langle(\Delta w_i)^2\rangle = \Delta t$

$$x_{i+1} = x_i + g(x_i)\Delta w_i + \frac{1}{2}g(x_i)g'(x_i)\Delta t$$

Equivalence of Ito and Stratonovich sde

Spurious drift term

Stratonovich sde

$$(S)\ dx = f(x)dt + g(x)dw(t)$$

is equivalent to an Ito sde

$$(I)\ dx = f(x)dt + \frac{1}{2}g(x)\partial_x g(x)dt + g(x)dw(t),$$

Change of variables: the Ito formula

Consider a general Ito stochastic equation

$$(I)\ dx = f(x)dt + g(x)dw(t), \quad (w(t)\dots \text{ Wiener process})$$

Forward Euler's method

$$\begin{aligned} x_{i+1} &= x_i + \Delta t f(x_i) + g(x_i)\Delta w_i, \quad (i = 0, 1, 2, 3, \dots) \\ \Delta w_i &= \sqrt{\Delta t} N(0, 1) \end{aligned}$$

What is the corresponding equation for $F(x(t))$?

Change of variables: the Ito formula

Differentiation chain rule (works in Ito interpretation only!)

$$
\begin{aligned}
dF[x(t)] &= F[x(t) + dx(t)] - F[x(t)] \\
&= F'[x(t)]dx(t) + \frac{1}{2}F''[x(t)]dx(t)^2 + \ldots \\
&= F'[x(t)]\left\{f(x)dt + g(x)dw(t)\right\} \\
&+ \frac{1}{2}F''[x(t)]\left\{f(x)dt + g(x)dw(t)\right\}^2 .
\end{aligned}
$$

To the order of $dw(t) \sim \sqrt{dt}$ and dt

$$
dF[x(t)] = \left\{f(x)F'[x] + \frac{1}{2}g(x)^2F''[x]\right\}dt + g(x)F'[x]dw(t).
$$

Change of variables in Stratonovich interpretation

Stratonovich sde

$$(S)\ dx = f(x)dt + g(x)dw(t)$$

Chain rule for depterministic functions

$$(S)\ dF(x(t)) = F'(x(t))dx = F'(x(t))(f(x)dt + g(x)dw)$$

Heun's method for Stratonovich sde

Example

Show that a Stratonovich sde

$$(S)\ dw = f(x)dt + g(x)dw(t)$$

can be integrated using Heun's method:

$$\begin{aligned} y_i &= x_i + f(x_i)\Delta t + g(x_i)\Delta w_i, \\ x_{i+1} &= x_i + \frac{1}{2}\left(f(x_i) + f(y_i)\right)\Delta t + \frac{1}{2}\left(g(x_i) + g(y_i)\right)\Delta w_i, \\ \Delta w_i &= N(0,1)\sqrt{\Delta t} \end{aligned}$$

Connection between the Fokker-Planck equation and a stochastic sde

For an Ito sde

$$(I)\ dx = f(x) + g(x)dw$$

Using Ito's change of variables formulae

$$\begin{aligned} & \langle dF(x(t))\rangle \\ = & \left\langle F'[x(t)]\left\{f(x)dt + g(x)dw(t)\right\} + \frac{1}{2}F''[x(t)]\left\{f(x)dt + g(x)dw(t)\right\}^2\right\rangle \end{aligned}$$

Using

$$\langle dw(t)\rangle = 0, \quad \langle g(x(t))F'(x(t))dw(t)\rangle = 0$$

$$\langle dF(x(t))\rangle = \left\langle f(x)F'(x) + \frac{1}{2}g^2(x)F''(x)\right\rangle dt,$$

Connection between the Fokker-Planck equation and a stochastic sde

In terms of the distribution function $p(x, t|x_0, t_0)$

$$\frac{\langle dF(x(t))\rangle}{dt} = \langle\frac{dF(x(t))}{dt}\rangle = \frac{d}{dt}\langle F(x(t))\rangle$$

$$= \int dx F(x)\partial_t p = \int dx \left[f(x)\partial_x F + \frac{1}{2}g(x)^2\partial_x^2 F\right] p$$

Integration by parts

$$\int dx F(x)\partial_t p = \int dx F(x)\left[-\partial_x(f(x)p) + \frac{1}{2}\partial_x^2(g(x)^2 p)\right].$$

Connection between the Fokker-Planck equation and a stochastic sde

The Fokker-Planck equation for the distribution $p(x,t|x_0,t_0)$

$$\begin{aligned} 0 &= \partial_t p + \partial_x J(x) \\ J(x) &= f(x)p - \frac{1}{2}\partial_x (g(x)^2 p) \end{aligned}$$

$J(x)\ldots$ the probability current

The Fokker-Planck equation for a Stratonovich sde

For a Stratonovich sde

$$(S)\ dx = f(x)dt + g(x)dw$$

The Fokker-Planck equation

$$\begin{aligned}
\partial_t p + \partial_x \left[f(x)p + \frac{1}{2} g(x) g'(x) p - \frac{1}{2}\partial_x (g(x)^2 p) \right] &= 0 \\
\partial_t p + \partial_x \left[f(x)p - \frac{1}{2} g(x) \partial_x (g(x) p) \right] &= 0
\end{aligned}$$

Fokker-Planck equation for a system of coupled SDEs

Set of n coupled equations

$$\dot{x}_i = f_i(x_1, x_2, \ldots, x_n) + \sum_{j=1}^{n} g_{ij}(x_1, x_2, \ldots, x_n)\xi_j(t), \quad (i = 1, 2, \ldots, n),$$

where $\xi_k(t)$ represent sources of uncorrelated white Gaussian noise.
In Stratonovich interpretation

$$\partial_t p = -\partial_i(f_i p) + \frac{1}{2}\partial_i \left(g_{im}\partial_k g_{km} p\right).$$

(sum over repeated indices)

Diffusion coefficient of a classical Brownian particle

One-dimensional motion of a particle m in a gas

$$\begin{aligned} \dot{x} &= \frac{p}{m} \\ \dot{p} &= -\alpha p + \sqrt{2D}\xi(t), \end{aligned}$$

Parameters $\alpha \ldots$ damping coefficient
$D \ldots$ characteristic strength of fluctuations
The Fokker-Planck equation

$$\begin{aligned} \partial_t \rho(x,p,t) &= -\partial_x \left(\frac{p}{m} \rho \right) + \partial_p [\alpha p \rho + D \partial_p \rho] \\ \partial_t \rho(x,p,t) &+ \partial_x J_x + \partial_p J_p = 0 \end{aligned}$$

Probability current $\boldsymbol{J} = (J_x, J_p)$

Diffusion coefficient of a classical Brownian particle

Stationary distribution

$$\begin{aligned}\partial_t \rho &= 0 \;\Rightarrow\; J_p = 0,\;\; J_x = f(p) \\ \rho_s &= \sqrt{\frac{\alpha}{2\pi D}}\exp\left(-\frac{\alpha p^2}{2D}\right).\end{aligned}$$

Spatially homogeneous distribution

Note that $\rho_s(p)$ does not depend on x. Distribution density can only be normalized on a finite interval X:

$$\int_X dx \int_{-\infty}^{\infty} \rho_s(p)\, dp = 1.$$

In what follows we set $X = 1$.

Diffusion coefficient of a classical Brownian particle

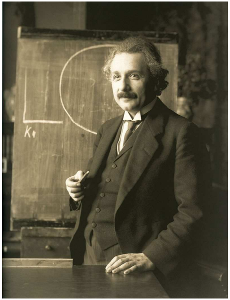
Maxwell's velocity distribution at temperature T

$$\rho_s(v) = \sqrt{\frac{m}{2\pi kT}} \exp\left(-\frac{mv^2}{2kT}\right)$$

Einstein's condition

$$D = \alpha mkT.$$

Albert Einstein (1879-1955)



Diffusion coefficient of a classical Brownian particle

Diffusion coefficient in 1D

$$D_\infty = \lim_{t\to\infty} \frac{\langle (x(t)-x(0))^2\rangle}{2t} = \lim_{t\to\infty} \frac{\langle x(t)^2\rangle - 2x(0)\langle x(t)\rangle + x(0)^2}{2t}.$$

We need to derive and solve the equations for time-dependent moments

$$\langle x(t)\rangle \text{ and } \langle x(t)^2\rangle$$

Diffusion coefficient of a classical Brownian particle

Taking the ensemble average of the Langevin equation

$$\begin{aligned}\partial_t\langle x(t)\rangle &= \langle \dot{x}\rangle = \frac{\langle p\rangle}{m}\\ \partial_t\langle p(t)\rangle &= \langle \dot{p}\rangle = -\alpha\langle p\rangle + \sqrt{2D}\langle\xi(t)\rangle = -\alpha\langle p\rangle\end{aligned}$$

Note that

$$\langle\xi(t)\rangle = 0$$

Diffusion coefficient of a classical Brownian particle

Ensemble average $\langle x(t)^2 \rangle$

$$\partial_t \langle x(t)^2 \rangle = 2\langle x(t)\dot{x}(t)\rangle = 2\frac{\langle x(t)p(t)\rangle}{m}$$

Ensemble average $\langle x(t)p(t) \rangle$

$$\begin{aligned}\partial_t \langle x(t)p(t)\rangle &= \langle x(t)\dot{p}(t)\rangle + \langle \dot{x}(t)p(t)\rangle \\ &= \langle x(t)[-\alpha p(t) + \sqrt{2D}\xi(t)]\rangle + \langle [p(t)/m]p(t)\rangle \\ &= -\alpha\langle x(t)p(t)\rangle + \langle p(t)^2\rangle/m\end{aligned}$$

Note that $\langle x(t)\xi(t)\rangle = 0$

Diffusion coefficient of a classical Brownian particle

Ensemble average $\langle p(t)^2 \rangle$

$$\begin{aligned} \partial_t \langle p(t)^2 \rangle &= 2\langle p(t)\dot{p}(t) \rangle \\ &= 2\langle [-\alpha p(t)^2 + \sqrt{2D} p(t)\xi(t)] \rangle \end{aligned}$$

Momentum and noise are correlated

$$\langle p(t)\xi(t) \rangle \neq 0$$

Diffusion coefficient of a classical Brownian particle

Marginal distribution of the momentum $\Pi = \int_X \rho(x, p, t | x_0, p_0, t_0)\, dx$

$$\partial_t \Pi = -\int_X dx \left[\partial_x J_x + \partial_p J_p\right] = \partial_p(\alpha p \Pi + D \partial_p \Pi)$$

Ensemble average $\langle p(t)^2 \rangle$

$$\begin{aligned}
\partial_t \langle p(t)^2 \rangle &= \int p^2 \partial_t \Pi(p, t)\, dp = \int dp p^2 \partial_p(\alpha p \Pi + D \partial_p \Pi) \\
&= -\int dp 2\alpha p^2 \Pi - 2D \int dp\, p\, \partial_p \Pi \\
&= -2\alpha \langle p(t)^2 \rangle + 2D \int dp \Pi = -2\alpha \langle p(t)^2 \rangle + 2D
\end{aligned}$$

Diffusion coefficient of a classical Brownian particle

Correlation between momentum and noise

$$\langle p(t)\xi(t)\rangle = \sqrt{\frac{D}{2}}$$

Diffusion coefficient of a classical Brownian particle

Solution with initial conditions $x(t=t_0)=x_0$ **and** $p(t=t_0)=p_0$

$$
\begin{aligned}
\langle p(t)\rangle &= p_0 e^{-\alpha(t-t_0)}\\
\langle p(t)^2\rangle &= \frac{D}{\alpha}\left(1-e^{-2\alpha(t-t_0)}\right)+p_0^2 e^{-2\alpha(t-t_0)}\\
\langle x(t)\rangle &= x_0+\frac{p_0}{\alpha m}\left(1-e^{-\alpha(t-t_0)}\right)\\
\langle x(t)p(t)\rangle &= \frac{D}{\alpha^2 m}-\left(\frac{p_0^2}{\alpha m}-\frac{D}{\alpha^2 m}\right)e^{-2\alpha(t-t_0)}\\
&+\left((xp)_0-\frac{2D}{\alpha^2 m}+\frac{p_0^2}{\alpha m}\right)e^{-\alpha(t-t_0)}\\
\langle x(t)^2\rangle &= \frac{2Dt}{(\alpha m)^2}+C_1 e^{-\alpha(t-t_0)}+C_2 e^{-2\alpha(t-t_0)}.
\end{aligned}
$$

Diffusion coefficient of a classical Brownian particle

In the limit $t \to \infty$

$$D_\infty = \frac{D}{(\alpha m)^2} = \frac{kT}{\alpha m}$$

Particle mobility and Einstein's relation

Mobility of a particle

$$\mu = \frac{\text{velocity}}{\text{force}} = (\alpha m)^{-1}$$

$$D_\infty = \frac{D}{(\alpha m)^2} = \frac{kT}{\alpha m} = \mu kT.$$

Overdamped motion

Brownian particle in the limit of large friction

$$\dot{x} \quad = \quad \mu \times \text{force} + \text{noise} = -\mu \partial_x U(x) + \sqrt{2A}\xi(t)$$

$$\begin{aligned} U(x) \quad \ldots & \qquad \text{potential energy} \\ \mu \quad \ldots & \qquad \text{mobility} \end{aligned}$$

Fokker-Planck equation

$$\partial \rho + \partial_x [-\mu \partial U(x) \rho - A \partial_x \rho] = 0$$

Stationary zero current solution

$$\rho_s(x) = C \exp\left(\frac{-\mu U(x)}{A}\right), \;\; C = \left(\int_{-\infty}^{\infty} dx \, \exp\left(\frac{-\mu U(x)}{A}\right)\right)^{-1}$$

Overdamped motion

Equilibrium Boltzmann distribution

$$\rho_s \sim \exp\left(\frac{-U(x)}{kT}\right)$$

This implies

$$A = \mu kT$$

Special case: the barometric formula

Overdamped particle in the gravity field

$$U(x) = mgz, \Rightarrow \ \rho_s(z) \sim \exp\left(\frac{-mgz}{kT}\right)$$

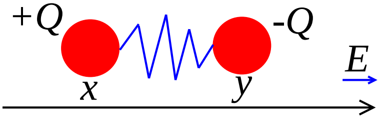
Pressure P of an ideal gas

$$P = \frac{\rho RT}{M}$$

$M \ldots$ Molar weight
$R \ldots$ gas constant
$\rho \ldots$ density
Barometric formulae

$$P = P_0 \exp\left(\frac{-Mgz}{RT}\right)$$

Bipolar molecule in external electric field



Coordinates of the two heads of the dimer x and y

$$
\begin{aligned}
\dot{x} &= \mu[-\alpha(x-y)+QE]+\sqrt{2\mu kT}\xi_x(t), \\
\dot{y} &= \mu[-\alpha(y-x)-QE]+\sqrt{2\mu kT}\xi_y(t)
\end{aligned}
$$

$Q \ldots$ electric charge
$E \ldots$ electric field
$\mu \ldots$ mobility of a single head
$\alpha \ldots$ spring constant (Hooke's law $U=\alpha(x-y)^2/2$)
$\xi_x(t),\ \xi_y(t) \ldots$ independent sources of white Gaussian noise

Bipolar molecule in external electric field

Transformation to new variables
$U = \frac{x+y}{2} \ldots$ center of mass coordinate
$V = x - y \ldots$ $(\pm)$ the diameter of the dimer
Langevin equations for U and V

$$\begin{aligned}\dot{U} &= \sqrt{2\mu kT}\frac{\xi_x(t)+\xi_y(t)}{2}, \\ \dot{V} &= -2\mu\alpha V + 2\mu QE + \sqrt{2\mu kT}(\xi_x(t)-\xi_y(t))\end{aligned}$$

Bipolar molecule in external electric field

Sum of two Gaussian white noise terms

Linear combination of two independent Gaussian white noise terms is also a Gaussian white noise with modified variance

$$\begin{aligned} \xi_x(t) + \xi_y(t) &= \eta(t) \\ \xi_x(t) - \xi_y(t) &= \chi(t), \end{aligned}$$

with

$$\langle \eta(t)\eta(t') \rangle = \langle (\xi_x(t) + \xi_y(t))(\xi_x(t') + \xi_y(t')) \rangle = 2\delta(t - t')$$
$$\langle \chi(t)\chi(t') \rangle = \langle (\xi_x(t) - \xi_y(t))(\xi_x(t') - \xi_y(t')) \rangle = 2\delta(t - t')$$

Bipolar molecule in external electric field

Langevin equations for U and V

$$\begin{aligned}\dot{U} &= \sqrt{\mu k T}\xi_U(t),\\ \dot{V} &= -2\mu\alpha V + 2\mu Q E + \sqrt{4\mu k T}\xi_V(t),\end{aligned}$$

with two independent Wiener processes

$$dw_U = \xi_U(t)dt,\ dw_V = \xi_V(t)dt$$

Relation to Ornstein-Uhlenbeck process

Equation for V is reduced to the Ornstein-Uhlenbeck process by the change of variables

$$\hat{V} = V - \frac{QE}{\alpha}$$

Bipolar molecule in external electric field

Dimer diffusion coefficient

$$D = \lim_{U \to \infty} \frac{\langle (U - U_0)^2 \rangle}{2t} = \frac{\mu k T}{2}$$

Example

Show that the diffusion coefficient of a centre of mass of N overdamped identical particles is

$$D = \frac{\mu k T}{N}$$

Bipolar molecule in external electric field

Langevin equation for $\hat{V}$

$$\dot{\hat{V}} = -2\mu\alpha\hat{V} + \sqrt{4\mu kT}\xi_V(t)$$

Recall the stationary zero current solution for the Orstein-Uhlenbeck process

$$\rho_s(\hat{V}) = \sqrt{\frac{\alpha}{2\pi kT}} \exp\left(\frac{-\alpha\hat{V}^2}{2kT}\right)$$

Bipolar molecule in external electric field

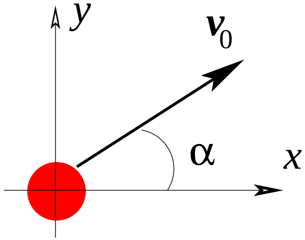
Average dipole moment

$$Q\langle V\rangle = \frac{Q^2 E}{\alpha}$$

Average size (diameter) of the dimer

$$\begin{aligned} s &= \sqrt{\langle (V - \langle V\rangle)^2\rangle} = \sqrt{\langle \hat{V}^2\rangle} \\ &= \sqrt{\frac{\alpha}{2\pi kT}} \int_{-\infty}^{\infty} d\hat{V}\, \hat{V}^2 \exp\left(\frac{-\alpha \hat{V}^2}{2kT}\right) \\ &= \frac{kT}{\alpha} \end{aligned}$$

Active Brownian particle



Motion in 2D

$$
\begin{aligned}
\dot{x} &= v_0 \cos\alpha + \sqrt{2\mu kT}\,\xi_x(t), \\
\dot{y} &= v_0 \sin\alpha + \sqrt{2\mu kT}\,\xi_y(t), \\
\dot{\alpha} &= \sqrt{2D_r}\,\eta(t)
\end{aligned}
$$

Active Brownian particle

Motion in 3D

$$\dot{\boldsymbol{r}} = v_0(z)\boldsymbol{p} + \boldsymbol{\xi}(t), \;\; \dot{\boldsymbol{p}} \;\; = \;\; \boldsymbol{\eta}(t) \times \boldsymbol{p},$$

with three-dimensional rotational noise

$$\boldsymbol{\eta}(t) = (\eta_x(t), \eta_y(t), \eta_z(t)).$$

Fokker-Planck equation in the Stratonovich interpretation

$$\partial_t \rho = D\mathbf{R}^2 \rho,$$

with

$$\mathbf{R} = \boldsymbol{p} \times \nabla_p = (p_x, p_y, p_z) \times (\partial_{p_x}, \partial_{p_y}, \partial_{p_z})$$

(M. Enculescu and H. Stark, *Active Colloidal Suspensions Exhibit Polar Order under Gravity*, Phys. Rev. Lett. **107**, 058301 (2011))