Nonequilibrium Field Theories and Stochastic Dynamics

Zehong Liao

December 8, 2025

1 From Ensemble to Trajectory: Retrospect and New Perspective

Whether it is the Master Equation or the Fokker-Planck Equation, they both answer the question: "Where is the particle **likely** to be at time t?" However, they do not directly answer the question: "How did a **specific** particle move from time 0 to time t?". The trajectory we observe for a single Brownian particle is a continuous, nowhere-differentiable, and unpredictable path.

The Langevin equation, proposed in 1908 by the French physicist Paul Langevin, was initially used to describe the irregular motion of suspended particles in a fluid caused by molecular collisions, laying the foundation for statistical mechanics and stochastic process research. At its core, it is a stochastic differential equation that describes the dynamical behavior of a microscopic particle subjected to a potential field, friction, and random noise (Gaussian noise), thereby satisfying the fluctuation-dissipation theorem and revealing the process by which a system moves from a non-equilibrium state towards thermal equilibrium.

The applications of this equation are wide-ranging: from Brownian motion simulation and molecular dynamics research in physics, to reaction rate modeling in chemistry, and protein folding dynamics analysis in biology. Furthermore, it provides the theoretical framework for stochastic gradient descent algorithms in machine learning, and it is used for risk assessment and stock price fluctuation modeling in financial mathematics.

The transition from the Fokker-Planck equation to the Langevin equation is more than just a mathematical change; it represents a profound change in fundamental perspective. The Fokker-Planck equation itself describes the evolution of the probability distribution $P(x,t)$, which, given an initial distribution, is entirely deterministic. In contrast, the Langevin equation describes the trajectory $x(t)$ of a single particle, which is fundamentally **stochastic**. These two are not mutually exclusive but are two sides of the same coin: one describes the "how-to-evolve" of the pedestrian crowd, while the other describes the movement of every single step of a pedestrian. As we will see later, there is a deep and precise mathematical relationship between the parameters of the Langevin equation (driving and noise intensity) and the coefficients of the Fokker-Planck equation (drift and diffusion terms). Understanding this duality is key to mastering the theory of stochastic processes.

Let us begin with a concrete physical system: a microscopic particle suspended in a liquid, the classic **Brownian Particle**. The simplest modeling approach is to directly apply our familiar macroscopic physical theorems. An object moving in a viscous fluid experiences drag, and this drag is usually proportional to velocity (Stokes' drag). According to Newton's Second Law, we can write:

$$m\frac{dv(t)}{dt} = -m\xi v(t) \tag{1}$$

Here, m is the mass of the particle, and $v(t)$ is its velocity. The professor used $m\xi$ on his whiteboard to denote the friction coefficient, a quantity which is also commonly referred to as γ. Thus, $\gamma = m\xi$ is the friction coefficient describing the magnitude of the resistance. For a spherical particle with radius R, in a fluid with viscosity η, this coefficient is given by the Stokes formula:

$$\gamma = 6\pi\eta R \tag{2}$$

This is a simple first-order ordinary differential equation, the solution to which is:

$$v(t) = v_0 e^{-\xi t} \tag{3}$$

This model predicts that, regardless of the particle's initial velocity v_0, its velocity will decay exponentially to zero over a characteristic time scale of ξ^{-1}. This naive macroscopic model attempts to describe a system fundamentally dominated by microscopic randomness using classical, deterministic Newtonian mechanics. It correctly captured the key physical mechanism of "friction dissipating energy." However, the fundamental limitation of this model is that it completely neglects the random impacts caused by the thermal motion of the fluid molecules. It predicts the particle will stop, which contradicts the incessant Brownian motion actually observed under a microscope.

The conclusion of this simple model—that a particle in a liquid will eventually come to rest—is clearly at odds with our observations and physical intuition. A grain of pollen in a fluid at temperature T never truly "rests," but is always undergoing perpetual, irregular motion.

The key here lies in thermodynamics. According to the **Equipartition Theorem** in statistical mechanics, in a state of thermal equilibrium, the average energy of a system per degree of freedom is $\frac{1}{2}k_BT$. For a particle moving in three-dimensional space, it has three translational degrees of freedom, and thus its average kinetic energy is:

$$\langle E_{\text{kin}} \rangle = \frac{1}{2}m\langle v^2 \rangle = \frac{3}{2}k_BT \tag{4}$$

Here, k_B is the Boltzmann constant, and T is the absolute temperature of the environment. This basic physical requirement dictates that as long as the temperature $T > 0$, the mean-square velocity of the particle $\langle v^2 \rangle$ must be a non-zero constant. Its root-mean-square velocity, the **thermal velocity**, is:

$$\sqrt{\langle v^2 \rangle} = \sqrt{\frac{3k_BT}{m}} \tag{5}$$

This creates a sharp contradiction: the naive deterministic model predicts $v \to 0$, while the laws of thermodynamics assert that $\langle v^2 \rangle$ must maintain a non-zero value determined by the temperature.

To resolve this contradiction, Einstein proposed a brilliant hypothesis: besides the macroscopic viscous resistance, the particle also receives an additional, rapidly changing **random force**, denoted by $\eta(t)$. This force represents the constant, random collisions with countless surrounding liquid molecules.

By adding this random force to the equation of motion, we obtain the **Langevin equation**, which describes the velocity evolution of the Brownian particle:

$$m\frac{d\mathbf{v}(t)}{dt} = -m\xi\mathbf{v}(t) + \boldsymbol{\eta}(t) \tag{6}$$

This equation beautifully embodies the dual effect of the fluid on the Brownian particle:

1. **Dissipation:** Through the viscous resistance term $-m\xi\mathbf{v}(t)$, the fluid constantly consumes the kinetic energy of the particle, causing it to decelerate.
2. **Fluctuation:** Through the random force term $\boldsymbol{\eta}(t)$, the fluid constantly transmits its own heat (the energy of the molecules' random motion) to the particle, causing it to accelerate.

Introducing the random force $\boldsymbol{\eta}(t)$ is not a simple "patchwork" correction. It encompasses a profoundly subtle physical idea: the microscopic mechanisms that lead to **dissipation** (frictional force) and **fluctuation** (random force) are exactly the same. Both the frictional and random "kicks" originate from collisions between the particle and the fluid molecules. The macroscopic resistance $-m\xi\mathbf{v}(t)$ is the **average** effect of countless collisions received by the particle when it moves at a velocity $\mathbf{v}$; whereas the random force $\boldsymbol{\eta}(t)$ is the part of these collisions that **deviates from the average**. Therefore, dissipation and fluctuation are not independent physical phenomena; they are two sides of the same microscopic process—the average effect and the fluctuation effect. This realization is the core idea of the **fluctuation-dissipation theorem** that we will derive next.

2 fluctuation-dissipation theorem

- **Zero Mean** The probability of collision coming from any direction is equal, so the average effect of the random force is zero over a long time interval. This ensures that if we average over many trajectories, we can recover the deterministic equation of motion (without the random force). In mathematical language, this is expressed as:

$$\langle \boldsymbol{\eta}(t) \rangle = 0 \tag{7}$$

- **Delta-Correlated (White Noise):** The time scale of molecular collisions (picoseconds level) is much smaller than the typical time scale of the Brownian particle's motion (microseconds level or longer). Therefore, we can make an idealized assumption: the random forces at any two different moments are completely uncorrelated. This noise, which has no correlation in time, is called **Gaussian White Noise**.

The mathematical form of its **correlation function** is:

$$\langle \eta_i(t)\eta_j(t') \rangle = 2\Gamma \delta_{ij}\delta(t - t') \tag{8}$$

Let us explain this important formula term by term:

- $\boldsymbol{\Gamma}$: **Noise Strength**. It is a constant that describes how large the fluctuations of the random force are. Currently, its value is unknown.
- $\boldsymbol{\delta_{ij}}$: **Kronecker Delta** symbol. It indicates that it is 1 when $i = j$, and 0 otherwise. This means that the random force in the x direction is uncorrelated with the random force in the y or z direction.
- $\boldsymbol{\delta(t - t')}$: **Dirac Delta function**. It indicates that the random force is only correlated with itself at the identical instant $t = t'$, and the correlation is zero for any $t \neq t'$.

The Langevin equation is a linear stochastic differential equation. We can view it as a first-order ordinary differential equation driven by a random force $\eta(t)$. Its formal solution can be written as an integral equation:

$$v(t) = v_0 e^{-\xi t} + \frac{1}{m}\int_0^t d\tau e^{-\xi(t-\tau)}\eta(\tau) \tag{9}$$

For mathematical convenience, we introduce a standardized white noise $\boldsymbol{\lambda}(t) = \frac{1}{\sqrt{2\Gamma}}\boldsymbol{\eta}(t)$, whose correlation function is simpler: $\langle \lambda_i(t)\lambda_j(t') \rangle = \delta_{ij}\delta(t - t')$. Thus, the expression for the velocity can be written as:

$$v(t) = v_0 e^{-\xi t} + \frac{\sqrt{2\Gamma}}{m}\int_0^t d\tau e^{-\xi(t-\tau)}\lambda(\tau) \tag{10}$$

The Langevin equation is a linear stochastic differential equation. We can view it as a first-order ordinary differential equation driven by a random force $\eta(t)$. Its formal solution can be written as an integral equation:

$$v(t) = v_0 e^{-\xi t} + \frac{1}{m}\int_0^t d\tau e^{-\xi(t-\tau)}\eta(\tau)$$

The random force $\boldsymbol{\eta}(t)$ is assumed to be a form of **Gaussian White Noise**, characterized by two main properties:

- **Zero Mean (Zero Mean):** The probability of collision coming from any direction is equal, so the average effect of the random force is zero over a long time interval. This ensures that if we average over many trajectories, we can recover the deterministic equation of motion (without the random force). In mathematical language, this is expressed as:

$$\langle \boldsymbol{\eta}(t) \rangle = 0$$

- **Delta-Correlated (White Noise):** The time scale of molecular collisions (picoseconds level) is much smaller than the typical time scale of the Brownian particle's motion (microseconds level or longer). Therefore, we make an idealized assumption: the random forces at any two different moments are completely uncorrelated. This noise, which has no correlation in time, is called **Gaussian White Noise**.

The mathematical form of its **correlation function** is:

$$\langle \eta_i(t)\eta_j(t')\rangle = 2\Gamma\delta_{ij}\delta(t-t')$$

Let us explain this important formula term by term:

- $\boldsymbol{\Gamma}$: **Noise Strength**. It is a constant that describes how large the fluctuations of the random force are. Currently, its value is unknown.
- $\boldsymbol{\delta_{ij}}$: **Kronecker Delta** symbol. It indicates that it is 1 when $i=j$, and 0 otherwise. This means that the random force in the x direction is uncorrelated with the random force in the y or z direction.
- $\boldsymbol{\delta(t-t')}$: **Dirac Delta function**. It indicates that the random force is only correlated with itself at the identical instant $t=t'$, and the correlation is zero for any $t\neq t'$.

For mathematical convenience, we introduce a standardized white noise $\boldsymbol{\lambda}(t) = \frac{1}{\sqrt{2\Gamma}}\boldsymbol{\eta}(t)$, whose correlation function is simpler: $\langle \lambda_i(t)\lambda_j(t')\rangle = \delta_{ij}\delta(t-t')$. Thus, the expression for the velocity can be written as:

$$v(t) = v_0 e^{-\xi t} + \frac{\sqrt{2\Gamma}}{m}\int_0^t d\tau e^{-\xi(t-\tau)}\lambda(\tau)$$

Now, we consider the behavior of the system as it reaches **thermal equilibrium**. In the long-time limit ($t, t' \gg \xi^{-1}$), the system "forgets" its initial velocity v_0. The first term, which contains $e^{-\xi(t+t')}$, decays to zero, and we obtain the **steady-state velocity autocorrelation function**:

$$\langle v_i(t)v_j(t')\rangle_{\text{stat}} = \frac{\Gamma}{m^2\xi}\delta_{ij}e^{-\xi|t-t'|} \tag{11}$$

This result tells us that, even in the steady state, the velocity correlation does not completely vanish but decays exponentially with the time difference $|t-t'|$, where its characteristic time is the relaxation time ξ^{-1}.

The next step is crucial. We set $t=t'$ to obtain the mean-square velocity at any instant in the steady state:

$$\langle v_i(t)v_i(t)\rangle = \frac{\Gamma}{m^2\xi} \tag{12}$$

For three-dimensional space, the total mean-square velocity is the sum of the three components:

$$\langle v^2(t)\rangle = \sum_{i=1}^{3}\langle v_i(t)v_i(t)\rangle = 3\frac{\Gamma}{m^2\xi} \tag{13}$$

Finally, we equate the result derived from the Langevin dynamics model with the thermodynamic requirement obtained from the **Equipartition Theorem**, $\langle v^2\rangle = \frac{3k_BT}{m}$:

$$\frac{3\Gamma}{m^2\xi} = \frac{3k_BT}{m} \implies \Gamma = m\xi k_BT = \gamma k_BT$$

(where $\gamma = m\xi$ is the friction coefficient).

This is one of the core ideas of this lecture: the **Fluctuation-Dissipation Theorem (FDT)**.

The physical meaning of this theorem is profound: it clearly states that the noise strength Γ, which describes the amplitude of random fluctuations, is **not independent**. It is completely determined by two parameters we already know: the **dissipation (friction) coefficient** ($m\xi=\gamma$) and the **temperature** (T) describing the system's heat energy. Fluctuations and dissipation, these two seemingly opposing concepts, are linked together by a simple and universal relationship.

We have now fully described the velocity of the Brownian particle. Now, we turn to describing the change in its position, which is easier to observe experimentally.

The Langevin equation is a linear stochastic differential equation. We can view it as a first-order ordinary differential equation driven by a random force $\eta(t)$. Its formal solution can be written as an integral equation:

$$v(t) = v_0 e^{-\xi t} + \frac{1}{m}\int_0^t d\tau e^{-\xi(t-\tau)}\eta(\tau)$$

For mathematical convenience, we introduce a standardized white noise $\lambda(t) = \frac{1}{\sqrt{2\Gamma}}\eta(t)$, whose correlation function is simpler: $\langle \lambda_i(t)\lambda_j(t')\rangle = \delta_{ij}\delta(t-t')$. Thus, the expression for the velocity can be written as:

$$v(t) = v_0 e^{-\xi t} + \frac{\sqrt{2\Gamma}}{m}\int_0^t d\tau e^{-\xi(t-\tau)}\lambda(\tau)$$

The random force $\boldsymbol{\eta}(t)$ is assumed to be a form of **Gaussian White Noise**, characterized by two main properties:

- **Zero Mean (Zero Mean):** The probability of collision coming from any direction is equal, so the average effect of the random force is zero over a long time interval. This ensures that if we average over many trajectories, we can recover the deterministic equation of motion (without the random force). In mathematical language, this is expressed as:

$$\langle \boldsymbol{\eta}(t)\rangle = 0$$

- **Delta-Correlated (White Noise):** The time scale of molecular collisions (picoseconds level) is much smaller than the typical time scale of the Brownian particle's motion (microseconds level or longer). Therefore, we make an idealized assumption: the random forces at any two different moments are completely uncorrelated. This noise, which has no correlation in time, is called **Gaussian White Noise**.

The mathematical form of its **correlation function** is:

$$\langle \eta_i(t)\eta_j(t')\rangle = 2\Gamma\delta_{ij}\delta(t-t')$$

Let us explain this important formula term by term:

- $\boldsymbol{\Gamma}$: **Noise Strength**. It is a constant that describes how large the fluctuations of the random force are. Currently, its value is unknown.
- $\boldsymbol{\delta_{ij}}$: **Kronecker Delta** symbol. It indicates that it is 1 when $i = j$, and 0 otherwise. This means that the random force in the x direction is uncorrelated with the random force in the y or z direction.
- $\boldsymbol{\delta(t-t')}$: **Dirac Delta function**. It indicates that the random force is only correlated with itself at the identical instant $t = t'$, and the correlation is zero for any $t \neq t'$.

Now, we consider the behavior of the system as it reaches **thermal equilibrium**. In the long-time limit ($t, t' \gg \xi^{-1}$), the system "forgets" its initial velocity v_0. The first term, which contains $e^{-\xi(t+t')}$, decays to zero, and we obtain the **steady-state velocity autocorrelation function**:

$$\langle v_i(t)v_j(t')\rangle_{\text{stat}} = \frac{\Gamma}{m^2\xi}\delta_{ij}e^{-\xi|t-t'|}$$

This result tells us that, even in the steady state, the velocity correlation does not completely vanish but decays exponentially with the time difference $|t-t'|$, where its characteristic time is the relaxation time ξ^{-1}.

The next step is crucial. We set $t = t'$ to obtain the mean-square velocity at any instant in the steady state:

$$\langle v_i(t)v_i(t)\rangle = \frac{\Gamma}{m^2\xi}$$

For three-dimensional space, the total mean-square velocity is the sum of the three components and is given by:

$$\langle v^2(t)\rangle = \sum_{i=1}^{3}\langle v_i(t)v_i(t)\rangle = 3\frac{\Gamma}{m^2\xi}$$

Finally, we equate the result derived from the Langevin dynamics model with the thermodynamic requirement obtained from the **Equipartition Theorem**, $\langle v^2\rangle = \frac{3k_BT}{m}$:

$$\frac{3\Gamma}{m^2\xi} = \frac{3k_BT}{m} \implies \Gamma = m\xi k_BT = \gamma k_BT$$

(where $\gamma = m\xi$ is the friction coefficient).

This is one of the core ideas of this lecture: the **Fluctuation-Dissipation Theorem (FDT)**.

The physical meaning of this theorem is profound: it clearly states that the noise strength Γ, which describes the amplitude of random fluctuations, is **not independent**. It is completely determined by two parameters we already know: the **dissipation (friction) coefficient** ($m\xi = \gamma$) and the **temperature** (T) describing the system's heat energy. Fluctuations and dissipation, these two seemingly opposing concepts, are linked together by a simple and universal relationship.

The particle's displacement vector is defined as the integral of velocity over time:

$$\Delta x(t) = x(t) - x(0) = \int_0^t v(s)ds \tag{14}$$

The statistical quantity we are most interested in is the **Mean Squared Displacement (MSD)**, which is the ensemble average of the square of the displacement magnitude:

$$\langle|\Delta x(t)|^2\rangle = \left\langle \left(\int_0^t \mathbf{v}(s)ds\right) \cdot \left(\int_0^t \mathbf{v}(s')ds'\right) \right\rangle = \int_0^t ds \int_0^t ds' \langle \mathbf{v}(s) \cdot \mathbf{v}(s')\rangle \tag{15}$$

We substitute the steady-state velocity autocorrelation function into the integral. Utilizing the FDT $\Gamma = m\xi k_B T$, we have:

$$\langle \mathbf{v}(s) \cdot \mathbf{v}(s')\rangle = \sum_{i=1}^{3} \langle v_i(s) v_i(s')\rangle = 3\frac{\Gamma}{\xi m^2} e^{-\xi|s-s'|} \tag{16}$$

Substituting $\Gamma = m\xi k_B T$ into the equation above yields:

$$\langle \mathbf{v}(s) \cdot \mathbf{v}(s')\rangle = \frac{3k_B T}{m} e^{-\xi|s-s'|} \tag{17}$$

Substituting this expression back into the double integral and solving it, the final MSD expression is obtained after some calculation:

$$\langle|\Delta x(t)|^2\rangle = \frac{6k_B T}{m\xi}\left[t - \frac{1}{\xi}\left(1 - e^{-\xi t}\right)\right] \tag{18}$$

This MSD expression contains rich physical content. By analyzing its limits at different time scales, we can extract the two contrasting modes of Brownian motion.

Short Time Limit (Ballistic Motion) When the time t is much smaller than the velocity relaxation time ξ^{-1} ($t \ll \xi^{-1}$), we can use the Taylor series expansion for the exponential term: $e^{-\xi t} \approx 1 - \xi t + \frac{1}{2}(\xi t)^2 - \dots$. Substituting this into the MSD formula, we find:

$$\langle|\Delta x(t)|^2\rangle \approx \frac{6k_B T}{m\xi}\left[t - \frac{1}{\xi}\left(1 - (1 - \xi t + \frac{1}{2}(\xi t)^2)\right)\right] = \frac{3k_B T}{m} t^2 \tag{19}$$

Note that $\langle v^2\rangle = \frac{3k_B T}{m}$, thus $\langle|\Delta x(t)|^2\rangle \approx \langle v^2\rangle t^2$.

Physical Significance: In the very short time range, the particle has not had enough time and collisions with fluid molecules to change its direction and velocity. Its motion is primarily dominated by its own inertia, like a tiny bullet, and the displacement is proportional to the initial velocity multiplied by time. This motion is called **ballistic motion**, characterized by the MSD being proportional to t^2.

Long Time Limit (Diffusive Motion) When the time t is much larger than the velocity relaxation time ξ^{-1} ($t \gg \xi^{-1}$), the term $e^{-\xi t}$ approaches zero. The MSD formula simplifies to:

$$\langle|\Delta x(t)|^2\rangle \approx \frac{6k_B T}{m\xi}\left[t - \frac{1}{\xi}(1 - 0)\right] \approx \frac{6k_B T}{m\xi} t \tag{20}$$

In the long time range, the particle's initial velocity information has been completely randomized by countless random collisions. Its trajectory changes into a completely irregular, uncorrelated sequence of steps, also known as a **random walk**. This is the characteristic of **diffusive motion**, where the MSD is linearly proportional to time t.

The entire MSD curve is not just a mathematical result; it is an image that records the dynamical fingerprints of the particle's interaction with the environment. In a dual logarithmic plot of MSD versus time, the slope smoothly transitions from 2 in the short-time regime to 1 in the long-time regime. This change in slope reflects the transition of the dominant physical mechanism from inertia-dominated motion to friction-dominated motion. The time of this transition happens to be the velocity relaxation time $\tau_v = \xi^{-1} = m/\gamma$. Therefore, this curve vividly tells the complete story of the world transitioning from "inertia-dominated" to "friction-dominated".

In diffusion theory, the **diffusion coefficient** D is usually defined by the long-time behavior of the MSD. In d dimensions, its definition is:

$$\langle |\Delta x(t)|^2 \rangle = 2dDt \tag{21}$$

We compare this definition with the long-time limit result we derived in three dimensions ($d = 3$):

$$2(3)Dt = \frac{6k_BT}{m\xi}t \tag{22}$$

Eliminating $6t$ from both sides, we immediately obtain an extremely important relationship:

$$D = \frac{k_BT}{m\xi} = \frac{k_BT}{\gamma} \tag{23}$$

This is the famous **Stokes-Einstein Relation**. It connects a macroscopic transport property—the **diffusion coefficient** D (which describes how fast matter spreads)—with the system's microscopic features—the **temperature** T and the **friction coefficient** γ. This relationship is one of the cornerstones of statistical physics, enabling us to infer microscopic information, such as the size of molecules, by observing macroscopic diffusion phenomena.

3 Simulating Brownian particles using Python

Since the Langevin equation contains a random term $\eta(t)$ that we cannot predetermine, we cannot solve for a deterministic trajectory analytically like with ordinary differential equations. We must rely on numerical methods.

For Stochastic Differential Equations (SDEs), the simplest numerical integration method is the **Euler-Maruyama Method**. It is a direct generalization of the Euler method we are familiar with for solving ordinary differential equations. We discretize time and velocity variables, with a time step of Δt. The update rules for position and velocity are as follows:

$$x_{n+1} = x_n + v_n \Delta t \tag{24}$$

$$m(v_{n+1} - v_n) = -m\xi v_n \Delta t + \int_{t_n}^{t_{n+1}} \eta(\tau) d\tau \tag{25}$$

The key here lies in how to handle the noise integral term $\int_{t_n}^{t_{n+1}} \eta(\tau)d\tau$. Due to the delta-correlation property of white noise, the result of this integral is a random variable whose standard deviation scales not as Δt, but as $\sqrt{\Delta t}$. Specifically, this integral can be approximated by a Gaussian random number with a mean of 0 and a variance of $2\Gamma\Delta t$.

Therefore, the final iterative format for velocity is:

$$v_{n+1} = v_n - \xi v_n \Delta t + \frac{\sqrt{2\Gamma\Delta t}}{m} N(0, 1) \tag{26}$$

where $N(0, 1)$ is a random vector drawn from the standard normal distribution (mean 0, variance 1).

- **Short-time regime:** At short time scales (tll$tau = 1.0$s), the simulated data points (blue circles) coincide with the theoretical line (red solid line) having a slope of 2. This is characteristic of **ballistic motion**.

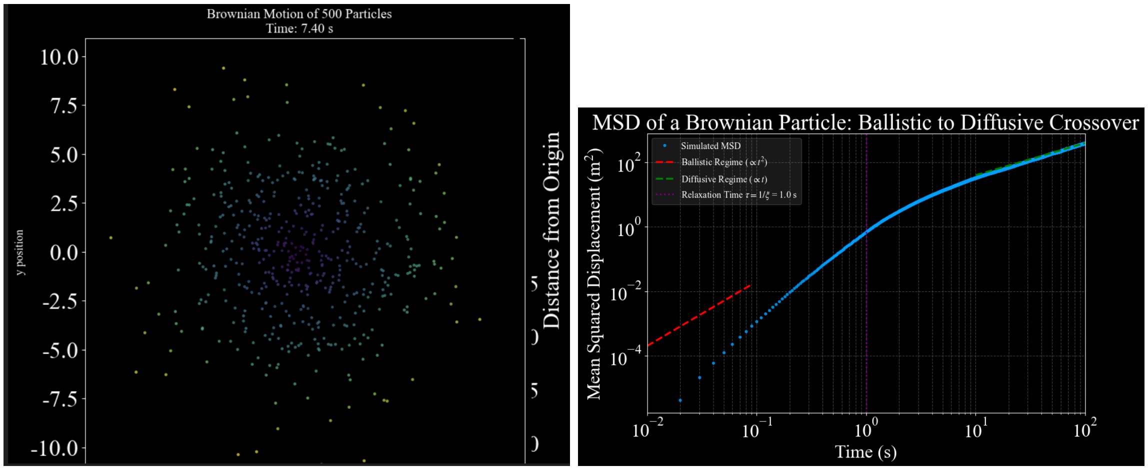

Figure 1: The MSD of all 500 simulated particles was calculated and plotted on a double logarithmic scale (log-log plot).

- **Long-time regime:** At long time scales (tggtau = 1.0s), the simulated data points coincide with the theoretical line (green dashed line) having a slope of 1. This is characteristic of **diffusive motion**.
- **Intermediate regime:** In the intermediate region, near the characteristic **relaxation time** $\tau = 1.0$s (marked by the purple dashed line), the simulation data smoothly transitions from one region to the other.

This computational experiment is merely a simple visualization. In the theoretical derivation, we utilized an **idealized model** that is not entirely physically realistic: the **delta-correlated white noise**. However, our numerical simulation, which is based on a discrete version of this idealized model (meaning the noise at each step is entirely **uncorrelated** with the previous step), successfully reproduces the complex physical phenomenon involving two different dynamical regimes.

This demonstrates that, even though the microscopic collisions have a limited **duration**, as long as the time scale of the **Brownian particle motion** we are interested in is much **greater than the collision time**, white noise serves as an **extremely effective and accurate physical model**.

4 Fock-Planck equations for velocity

We start with the Langevin equation for the velocity v of a free Brownian particle:

$$m\frac{dv}{dt} = -m\xi v(t) + \eta(t) \tag{27}$$

Let's perform a physical analysis of the terms in this equation:

- $m\frac{dv}{dt}$: The **inertia term**, which is mass times acceleration, according to Newton's second law.
- $-m\xi v(t)$: The **drag** or **damping force**, whose direction is always opposite to the direction of motion. Here, ξ is the friction coefficient per unit mass.
- $\eta(t)$: The **random force** (or **stochastic force**), representing continuous, random collisions from surrounding fluid molecules.

The statistical properties of the random force $\eta(t)$ are crucial. It is modeled as a **Gaussian distributed** random variable with the following properties:

- **Zero Mean Value:** $\langle \eta_i(t) \rangle = 0$. This indicates that, on average, the random collisions have no preferred direction.

- **Delta-Correlated Covariance (White Noise):** $\langle\eta_i(t)\eta_j(t')\rangle = 2\Gamma\delta_{ij}\delta(t-t')$. This is a mathematical idealization of the fluctuations. The Dirac delta function $\delta(t-t')$ means that the force at any instant is completely uncorrelated with the force at any other instant, no matter how close the two times are. The strength of these fluctuations is determined by Γ.

Here, the expression for Γ is $\Gamma = m\xi k_B T$. This is a profound result derived from a preceding discussion, and it is the very manifestation of the **Fluctuation-Dissipation Theorem** (FDT). This theorem connects the magnitude of the random fluctuations (described by Γ) with the energy dissipation of the system (described by the friction coefficient ξ) and the temperature of the heat bath (T). This connection is not accidental; it is a necessary condition for the system to eventually reach thermal equilibrium.

To analyze the statistical properties of the velocity change, we discretize the Langevin equation over a small time step Δt. This transforms the differential equation into an update rule:

$$m\frac{\Delta v}{\Delta t} = -m\xi v(t) + \frac{\Delta W(t,\Delta t)}{\Delta t} \tag{28}$$

(Note: The original image's presentation of the equation is slightly unusual for standard discretization, often $\Delta v = -\xi v(t)\Delta t + \frac{1}{m}\Delta W(t,\Delta t)$ is preferred, but I will strictly follow the provided image structure.)

We define the **Noise Increment** ΔW as the integral of the random force over this infinitesimal time interval:

$$\Delta W(t,\Delta t) := \int_t^{t+\Delta t} d\tau \eta(\tau) \tag{29}$$

This quantity represents the **net random impulse** received by the particle during the time Δt. Utilizing the statistical properties of $\eta(t)$, we can derive the mean and covariance of ΔW:

- **Mean:**

$$\langle\Delta W_i\rangle = \int_t^{t+\Delta t} d\tau\langle\eta_i(\tau)\rangle = 0.$$

- **Covariance:** According to the key calculation:

$$\langle\Delta W_k \Delta W_j\rangle = \int_t^{t+\Delta t} d\tau \int_t^{t+\Delta t} d\tau' \langle\eta_k(\tau)\eta_j(\tau')\rangle = 2m\xi k_B T\delta_{kj}\Delta t \tag{30}$$

The variance of the noise increment $\langle(\Delta W)^2\rangle$ is proportional to Δt, and **not** to $(\Delta t)^2$. This is key to understanding the random process. A standard deterministic quantity, like displacement, is proportional to Δt for velocity, or $(\Delta t)^2$ for acceleration. However, the linearity of the variance of integrated noise with Δt is rooted in the **Delta-correlation (white noise)** of the noise $\eta(t)$. This mathematical characteristic is the root of the feature that displacement in Brownian motion scales with the square root of time, $\sqrt{\Delta t}$, which is also the essential difference between stochastic and ordinary integration.

Now, we introduce the concepts of the **drift coefficient** A_i and the **diffusion coefficient** B_{ij}, which are defined as the first and second moments of the velocity change per unit time, respectively. These two coefficients are the foundation for constructing the **Fokker-Planck equation**.

- **Definition:** $A_i = \lim_{\Delta t\to 0}\frac{\langle\Delta v_i\rangle}{\Delta t}$. It represents the average, deterministic "**drift**" or "**push**" experienced by the particle's velocity.

- **Derivation:** According to the video, we take the average of the discretized Δv_i equation:

$$\langle\Delta v_i\rangle = \langle -\xi v_i \Delta t + \frac{\Delta W_i}{m}\rangle = -\xi v_i \Delta t \tag{31}$$

  This is because the mean value of the noise increment is zero, i.e., $\langle\Delta W_i\rangle = 0$.

- **Result:** $A_i = -\xi v_i$. The physical meaning of this result is very clear: the average drift of the velocity is entirely caused by the **friction force**, which always tries to reduce the velocity, pushing it towards zero.

- **Definition:** $B_{ij} = \lim_{\Delta t \to 0} \frac{\langle \Delta v_i \Delta v_j \rangle}{\Delta t}$. It represents the variance of the velocity fluctuations, quantifying the degree to which the probability distribution "**diffuses**" in velocity space due to the effect of the random force.

- **Derivation:** Following the calculation in the course, we only retain the lowest order term in Δt in the limit $\Delta t \to 0$:

$$\langle \Delta v_i \Delta v_j \rangle = \left\langle \left(-\xi v_i \Delta t + \frac{\Delta W_i}{m} \right) \left(-\xi v_j \Delta t + \frac{\Delta W_j}{m} \right) \right\rangle \approx \frac{1}{m^2} \langle \Delta W_i \Delta W_j \rangle \tag{32}$$

  In the process of taking the limit, terms related to $(\Delta t)^2$ and $\Delta t \langle \Delta W \rangle$ will vanish.

- **Result:** $B_{ij} = \frac{1}{\Delta t} \frac{1}{m^2} (2m\xi k_B T \delta_{ij} \Delta t) = \frac{2k_B T \xi}{m} \delta_{ij}$. This result shows that the diffusion in velocity space is constant, and its strength is directly proportional to the temperature of the environment.

When the time is long enough ($t \to \infty$), the system reaches **equilibrium**, at which point the probability distribution no longer changes with time, i.e., $\partial_t p = 0$. This means the probability flux caused by drift and diffusion must exactly cancel each other out.

The solution to this steady-state equation is:

$$p_{eq}(v) \propto \exp\left(-\frac{mv^2}{2k_B T} \right) \tag{33}$$

This is an extremely profound result. We started from a purely dynamic model (**Langevin equation**), a model that knows nothing about statistical mechanics or thermodynamics. By deriving and solving the **Fokker-Planck equation**, we proved that this dynamic model will naturally lead to the velocity's **Maxwell-Boltzmann distribution**, which is the cornerstone of equilibrium statistical mechanics.

The Langevin equation describes the cause (friction and random collisions), the Fokker-Planck equation describes the process (drift and diffusion of probability), and the Maxwell-Boltzmann distribution is the final result (the unique, stable equilibrium state). The Fokker-Planck equation provides a dynamic mechanism for a system to heat up through interaction with the environment (friction and fluctuations), ultimately reaching the equilibrium state predicted by thermodynamics. In this process, the **Fluctuation-Dissipation Theorem** ($\Gamma \propto \xi T$) is the key guarantee that the system can reach the correct equilibrium. Without it, the balance between drift and diffusion would be broken, and the system would not spontaneously relax to the correct state determined by the temperature T.

5 Overdamped limit and Smolenshowski equation

Now, we extend the system under study from a free particle to a particle moving in a potential field $U(x)$. The complete Langevin equation for this is:

$$m\frac{d^2x}{dt^2} + m\xi \frac{dx}{dt} = -\nabla U(x) + \eta(t) \tag{34}$$

We can clearly identify the terms in the equation: the inertia term, the damping term, the conservative force term, and the random force term.

In many physical and biological systems, such as colloidal particles in water or proteins in cytoplasm, the damping force ($m\xi \frac{dx}{dt}$) is much larger than the inertia term ($m\frac{d^2x}{dt^2}$). In this "**overdamped**" or "**high friction**" limit, the particle's momentum is rapidly randomized due to frequent collisions, allowing its velocity to adapt instantaneously to the local force field.

This approximation is a classic example of **timescale separation**. The velocity v is a "**fast variable**" that relaxes to its steady state on a very short timescale, $1/\xi$. The position x is a "**slow variable**" that changes over a much longer period. By assuming the velocity reaches equilibrium instantaneously, we can derive a simpler, effective equation of motion. In other words, in the overdamped limit, we no longer care about the fast fluctuations of the velocity v around its equilibrium, only the slow evolution of the particle's position x caused by them.

By setting the inertia term $m\frac{d^2x}{dt^2}$ to zero, we obtain the **Overdamped Langevin Equation**, also known as the Smoluchowski-Langevin Equation:

$$m\xi\frac{dx}{dt} = -\nabla U(x) + \eta(t) \tag{35}$$

We can now rearrange the aforementioned equation into a more standard form:

$$\frac{dx}{dt} = -\frac{1}{m\xi}\nabla U(x) + \frac{1}{m\xi}\eta(t) = -\mu\nabla U(x) + \xi(t) \tag{36}$$

Here, we define the **mobility** $\mu := \frac{1}{m\xi}$. It represents the terminal velocity the particle achieves under a unit external force.

The new noise term $\xi(t) = \frac{1}{m\xi}\eta(t)$ has new statistical properties. Its covariance is:

$$\langle \xi_i(t)\xi_j(t')\rangle = \frac{\langle \eta_i(t)\eta_j(t')\rangle}{(m\xi)^2} = \frac{2m\xi k_B T}{(m\xi)^2}\delta_{ij}\delta(t-t') = 2\frac{k_B T}{m\xi}\delta_{ij}\delta(t-t') \tag{37}$$

Typically, we define the **diffusion coefficient** D by the noise strength: $\langle \xi_i(t)\xi_j(t')\rangle = 2D\delta_{ij}\delta(t-t')$. By comparing these two expressions, we obtain the famous **Einstein Relation**:

$$D = \mu k_B T \tag{38}$$

This relationship is highly significant, as it connects a macroscopic transport coefficient (D), which describes the speed of particle diffusion, with the microscopic particle response to force (μ) and the thermal energy ($k_B T$).

The derivation of the **Einstein Relation** $D = \mu k_B T$ originated from Einstein's theoretical research on Brownian motion in 1905, and Marian Smoluchowski's independent derivation in 1906. The core idea is that the random motion (diffusion) in thermal equilibrium and the directional motion (drift) driven by an external field are both governed by the thermal energy $k_B T$. This equation is not only an early manifestation of the **Fluctuation-Dissipation Theorem**, but also provides a theoretical foundation for subsequent research. The Einstein relation unifies microscopic fluctuations and macroscopic response, serving as a key bridge for statistical physics and engineering applications.

Now, we repeat the derivation process for the Fokker-Planck equation, but this time for the **position variable** x, using the **Overdamped Langevin Equation**.

- **Drift Coefficient** A_i**:**

$$A_i = \lim_{\Delta t\to 0}\frac{\langle \Delta x_i\rangle}{\Delta t} = \langle -\mu\partial_i U\rangle = -\mu\partial_i U = \mu F_i \tag{39}$$

  The drift here is determined by the **conservative force** $F = -\nabla U$.

- **Diffusion Coefficient** B_{ij}**:**

$$B_{ij} = \lim_{\Delta t\to 0}\frac{\langle \Delta x_i \Delta x_j\rangle}{\Delta t} = \frac{1}{\Delta t}\langle (\Delta W_\xi)_i(\Delta W_\xi)_j\rangle = 2D\delta_{ij} \tag{40}$$

  The diffusion in position space is **constant** (if D is constant), and its magnitude is given by the **diffusion coefficient** D.

Combining these coefficients, we obtain the **Smoluchowski Equation**, which describes the probability distribution $P(x,t)$ in position space, and is the Fokker-Planck equation for position space:

$$\partial_t P(x,t) = \nabla\cdot[\mu P(\nabla U)P(x,t)] + D\nabla^2 P(x,t) \tag{41}$$

This equation can also be written as: $\partial_t P = \nabla\cdot[\mu(\nabla U)P + D\nabla P]$.

We can simply set $\partial_t P = 0$ to solve for the equilibrium state. This means the probability flux due to drift and diffusion must exactly cancel each other out.

The solution to this steady-state equation is:

$$P_{eq}(x) \propto \exp\left(-\frac{U(x)}{k_B T}\right) \tag{42}$$

This is the **Boltzmann distribution** (Boltzmann Distribution), which is the fundamental hypothesis of classical statistical mechanics.

The Fokker-Planck equation provides a dynamic mechanism for the Boltzmann distribution. It tells us that for a system coupled to a thermal bath at temperature T, the thermal energy $k_B T$ drives fluctuations, which cause the particle to spread out in the potential $U(x)$, while the potential $U(x)$ creates a force that pushes the particle towards lower energy states.

In this precise balance, the potential $U(x)$ produces an average force pushing the particle towards lower energy regions, and the temperature-induced noise (random force) creates diffusion that spreads the particle throughout the space. The **Einstein Relation** ensures that the diffusion generated by the thermal noise perfectly balances the drift generated by the force, resulting in the correct **Boltzmann distribution**

$$P_{eq}(x) \propto \exp\left(-\frac{U(x)}{k_B T}\right) \tag{43}$$

The **Boltzmann distribution** $P_{eq}(x) \propto \exp\left(-\frac{U(x)}{k_B T}\right)$ is the cornerstone of statistical mechanics, and its profound significance is multi-faceted. It was first proposed by Ludwig Boltzmann in the 1870s, extending Maxwell's kinetic theory of gases from velocity space to energy space. Essentially, it is the probability distribution that maximizes entropy for a given mean energy. In 1902, Josiah Willard Gibbs formally established the theory within the framework of statistical mechanics, solidifying its mathematical foundation. In 1905, Einstein, through his theoretical study of Brownian motion, and by confirming the universality of this distribution via the **Fluctuation-Dissipation Theorem** ($D = \mu k_B T$), revealed the precise balance between maximum diffusion and maximum entropy.

In applications, the Boltzmann distribution permeates multiple disciplines:

- **Chemistry**: It explains the temperature dependence of reaction rates and equilibrium constants through the Arrhenius equation.
- **Materials Science**: It describes defects (vacancies, interstitials) in crystals.
- **Biophysics**: It guides conformation changes and energy landscapes of proteins.
- **Information Science**: It forms the core of models like the Boltzmann machine, which led to the development of deep learning algorithms.

The Boltzmann distribution provides a unified framework for phenomena ranging from quantum physics (e.g., the high-temperature limit of the Bose-Einstein and Fermi-Dirac distributions) to astrophysics (e.g., the dark matter distribution in galactic halos).

6 Visualizing the Smolenskowski process

For a general **ordinary differential equation (ODE)**, we can use the simple **Euler method** $x_{n+1} = x_n + f(x_n)\Delta t$ for numerical solution. However, for a **stochastic differential equation (SDE)**, this naive method is incorrect because it does not properly handle the scaling of the stochastic term.

The correct, and simplest, numerical method for solving SDEs is the **Euler–Maruyama method**. For an SDE of the form $dX = a(X)dt + b(X)dW$, the update rule is:

$$X_{n+1} = X_n + a(X_n)\Delta t + b(X_n)\sqrt{\Delta t}\mathcal{N}(0,1) \tag{44}$$

where $\mathcal{N}(0,1)$ is a random number drawn from the **standard normal distribution** with mean 0 and variance 1.

The key distinction here lies in the scaling of the **stochastic increment**, which is proportional to $\sqrt{\Delta t}$, and not Δt. This directly reflects the conclusion we previously derived theoretically: the **variance** of the noise increment is proportional to Δt. The Euler–Maruyama method is a direct application of this theoretical result in numerical computation.

We will simulate the **overdamped Langevin dynamics** of multiple non-interacting particles in two-dimensional space.

- **Potential Model:** To clearly illustrate the concept, we choose a simple **two-dimensional harmonic oscillator potential well**, whose potential energy function is $U(x, y) = \frac{1}{2}k(x^2 + y^2)$. This is a **central confining potential**, and the force it generates is $\mathbf{F} = -\nabla U = -k\mathbf{r}$, which always points towards the origin.

- **Discretization Equation:** Applying the **Euler–Maruyama method** to our two-dimensional system yields the update rule for each time step:

$$x_{n+1} = x_n - \mu k x_n \Delta t + \sqrt{2D\Delta t}\mathcal{N}_x(0, 1) \tag{45}$$

$$y_{n+1} = y_n - \mu k y_n \Delta t + \sqrt{2D\Delta t}\mathcal{N}_y(0, 1) \tag{46}$$

  Where $\mathcal{N}_x$ and $\mathcal{N}_y$ are two independent **standard normal random numbers**.

- **Simulation Parameters:** In the code, we will define the necessary parameters, including the number of particles **num_particles**, the mobility **mu**, the potential well strength **k**, the diffusion coefficient **D** (which is related to the temperature $\mathbf{k}_B\mathbf{T}$ via the **Einstein relation**), the time step **dt**, and the total number of simulation steps **num_steps**.

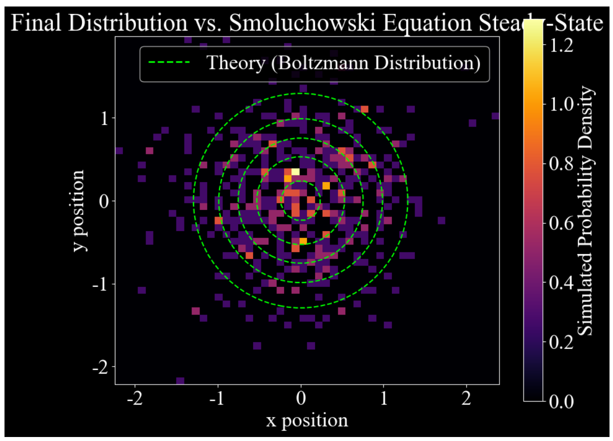

Figure 2:

This is a two-dimensional histogram generated from the final positions of all 500 particles at the end of the simulation, representing the **particle probability density** measured in the experiment or simulation. Overlaid on the heatmap are several concentric, smooth, green dashed circles. This represents the **theoretical prediction**. It is precisely calculated from the **steady-state solution** of the **Fokker-Planck equation**—the **Boltzmann distribution** $P_{eq}(\mathbf{x}) \propto \exp\left(-\frac{U(\mathbf{x})}{k_B T}\right)$—as contour lines of a two-dimensional Gaussian distribution. The statistical results (macroscopic view) from the long-term evolution of single-particle Langevin trajectories (microscopic view) converge exactly to the **steady-state solution** of the probability distribution described by the **Fokker-Planck-Boltzmann equation** (green contour lines).

7 Summary

1. **Statistical Law from Velocity Random Walk:** We start from the **complete Langevin equation** for velocity, which includes friction, noise, and inertia. By applying statistical analysis to the infinitesimal time interval (i.e., calculating its drift and diffusion coefficients), we can rigorously derive the evolution equation for the velocity probability density, the **Fokker-Planck equation**. The **steady-state solution** of this equation, as everyone knows, is the **Maxwell-Boltzmann distribution**. This validates the fundamental consistency between the Langevin model and statistical mechanics.

2. **Simplification under Overdamped Condition: The Smoluchowski Equation:** In many physical and biological systems (such as inside cells), the viscosity of the environment is extremely strong, causing the inertia of particles to become negligible. In this **overdamped limit**, the instantaneous velocity of the particle is largely determined by the forces acting on its current position. We then apply the mathematical tools of the Fokker-Planck equation again to the simplified, position **r**-describing Langevin equation, resulting in an evolution equation purely for the position probability density $P(\mathbf{x}, t)$—the **Smoluchowski Equation**.

3. **Equilibrium in a Potential Field:** The Smoluchowski equation describes the diffusion of particles in an external potential $U(\mathbf{x})$. Its steady-state solution is a fundamental result in statistical physics—the **Boltzmann distribution**:

$$P_{eq}(\mathbf{x}) \propto e^{-U(\mathbf{x})/k_B T}$$

   This result directly tells us that, after long-term evolution, particles are found more frequently in regions of lower potential energy. The Python model vividly reproduces this process: how particles evolve in the harmonic oscillator potential well and eventually form the profile of the **Boltzmann distribution**.

The physical law that runs through this entire derivation process is the **Fluctuation-Dissipation Theorem**. In this context, it is embodied by the **Einstein relation** $D = \mu k_B T$. It fundamentally illustrates that the 'agitation' driving particle motion (through the diffusion coefficient D and noise $\xi(t)$ in the system) and the system's resistance to motion and dissipation of energy (through the mobility μ or friction coefficient ζ) must establish a fixed ratio governed by the temperature T for the system to successfully reach thermal equilibrium.

Reference

- Nonequilibrium Field Theories and Stochastic Dynamics, Prof. Erwin Frey, LMU Munich, Summer Semester 2025
- Non-equilibrium States: Irreversibility and the Implications of Entropy Production — Non-equilibrium Field Theory and Stochastic Dynamics, Interesting Methods PhD
- https://mp.weixin.qq.com/s/6ZPccrywQRUKYNILhP49-Q

References