DIFFUSION PROCESS

THEORETICAL VIEW COMBINED WITH PYTHON CODE

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Abstract

This document explores the concept of Mean Squared Displacement as a fundamental tool for analyzing particle motion in various diffusion regimes. While mean squared displacement is often used to characterize normal diffusion, where it increases linearly with time, it is also crucial in identifying anomalous diffusion, where mean squared displacement follows different time behaviors.

The discussion begins with one-dimensional normal diffusion, demonstrating how mean squared displacement naturally emerges from both the Fokker–Planck Equation and its equivalent stochastic differential equation, which is subject to Brownian motion. The document then extends the discussion to two-dimensional normal diffusion and the general case of diffusion in d-dimensions.

Finally, it introduces anomalous diffusion, exploring how deviations from normal diffusion can be identified and analyzed using mean squared displacement.

1 Mean Squared Displacement

Let $r(t)$ be a random variable in $\mathbb{R}^d$, representing the position of a particle at time t. Its initial position at time $t = 0$ is denoted by r_0. The displacement vector, which describes how the particle has moved from its starting point, is given by $\vec{r}(t) - \vec{r_0}$.

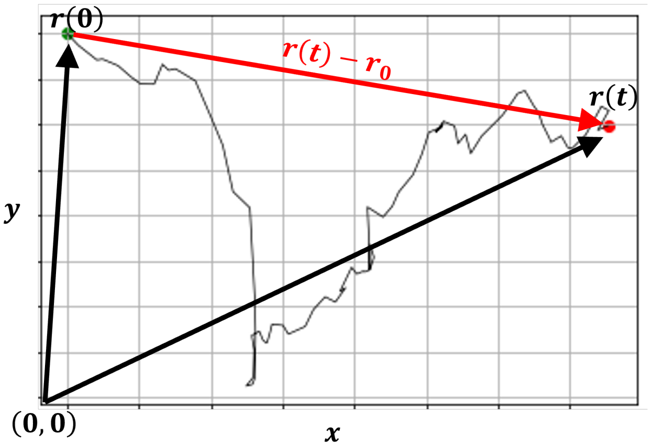


Figure 1.1:

This vector captures both the direction and magnitude of the motion. To quantify how far the particle has moved from its initial position, we compute the norm of the displacement vector

$$\|\vec{r}(t) - \vec{r_0}\| = \sqrt{\sum_{i=1}^{n} |x_i|^2}, \tag{1.1}$$

where x_i is the i-th component of the vector. To simplify the analysis and avoid dealing with square roots, we instead use the squared norm. Taking the expected value of the squared norm across many trajectories yields the Mean Squared Displacement. The Mean Squared Displacement (MSD), given by

$$\left\langle \|\vec{r}(t) - \vec{r_0}\|^2 \right\rangle, \tag{1.2}$$

is a measure used in physics, particularly in the study of particle motion and diffusion. It quantifies the average squared distance between the particle's position at time t and its initial position. MSD is crucial for understanding Brownian motion, diffusion processes, and the dynamics of particles in various systems. The analysis of MSD provides a quantitative measure of how particles diffuse or spread out over time, making it essential for understanding particle dynamics in various fields. The MSD is important because it reveals a lot about the statistical properties of the process[2, 3, 4].

2 Diffusion

In the context of a particle trajectory, diffusion refers to the process by which particles spread out over time due to random motion [2]. It can be observed in various fields, such as physical, chemical, and biological systems. A common way to quantify diffusion is by measuring the MSD of the particles over time [1]. In order to understand why, we need to understand the connection between Fokker-Planck Equation and stochastic differential equation.

2.1 Diffusion in 1D

In one-dimension, we can describe a diffusion process by Fokker-Planck Equation (FPE), also known as diffusion equation. In the case of pure random fluctuations, without any drift, the FPE is given by

$$\frac{\partial}{\partial t} p\left(x, t\right) = D \frac{\partial^2}{\partial x^2} p\left(x, t\right), \tag{2.1}$$

where $p\left(x, t\right)$ is a probability density function, x denotes the position, and t is time. The solution is a given by

$$p\left(x, t\right) = \frac{1}{\sqrt{4\pi D t}} e^{-\left(\frac{x}{\sqrt{4Dt}}\right)^2}, \tag{2.2}$$

which is a probability density function of a normally distributed random variable, whose variance grows linearly with time

$$x \sim \mathcal{N}\left(0, 2Dt\right). \tag{2.3}$$

This means that as time progresses, the variance increases, implying that the process is non-stationary, as its statistical properties change over time. The parameter D is called the diffusion coefficient. It quantifies the rate at which the particles diffuse and is important for understanding how quickly particles will spread [1, 2]. The larger the value of D, the faster the dispersion. Next, consider a stochastic differential equation (SDE) of the form

$$dx = \sqrt{2D}dB\left(t\right), \tag{2.4}$$

where $B\left(t\right)$ represents Brownian motion. This SDE describes the change in the particle's position due to pure random fluctuations of $B\left(t\right)$. It can be proved that FPE and this SDE are equivalent, namely

$$\frac{\partial p}{\partial t} = D\frac{\partial^2 p}{\partial x^2} \Longleftrightarrow dx = \sqrt{2D}dB\left(t\right), \tag{2.5}$$

meaning both equations describe the same process from different perspectives. Integrating the SDE with respect to time t yields

$$\begin{aligned} \int_0^t dx &= \sqrt{2D}\int_0^t dB\left(t\right) \\ \Longrightarrow x\left(t\right) - x_0 &= \sqrt{2D}B\left(t\right) \end{aligned} \tag{2.6}$$

where $x\left(0\right) = x_0$. The expectation is

$$\left\langle x\left(t\right) - x_0\right\rangle = \sqrt{2D}\left\langle B\left(t\right)\right\rangle = 0, \tag{2.7}$$

since the expectation of a Brownian motion at any time t is $\left\langle B\left(t\right)\right\rangle = 0$. Computing the variance gives

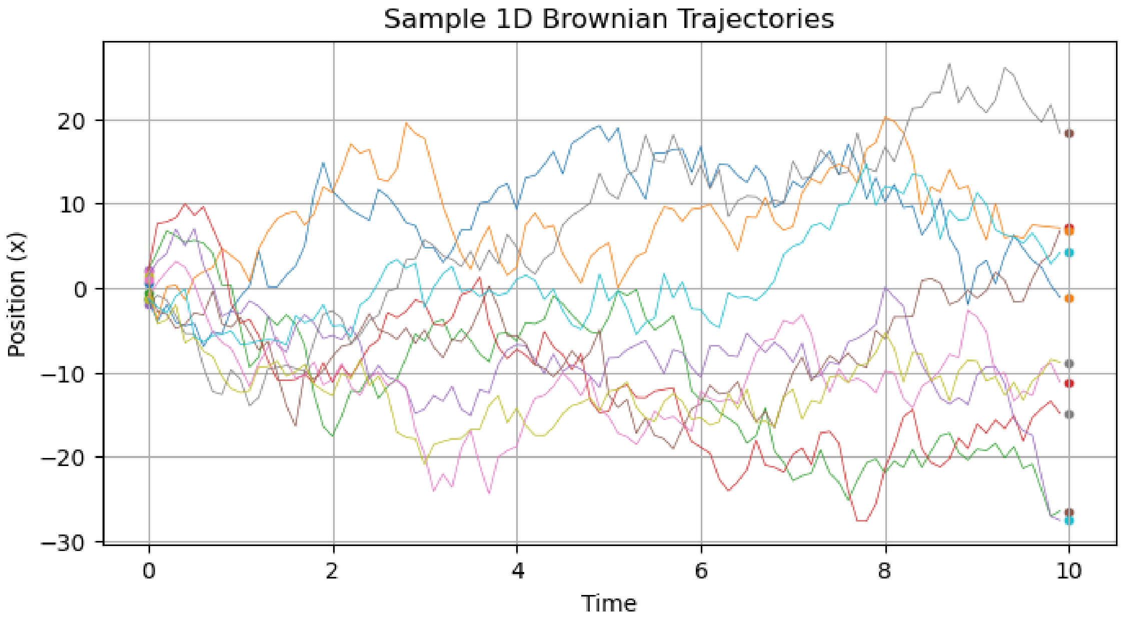
$$\left\langle \left(x\left(t\right) - x_0\right)^2\right\rangle = 2D\left\langle B^2\left(t\right)\right\rangle = 2Dt, \tag{2.8}$$

which is the same result obtained earlier from solving FPE. The left hand side is exactly what we defined as the MSD in one-dimension. Therefore, for simple diffusion, such as in the case of particles with trajectories subject to Brownian motion, we say that the MSD grows linearly with time t.

Simulation The following Python code demonstrates a simple one-dimensional diffusion process, computes the Mean Squared Displacement, and verifies its linear relationship with time.

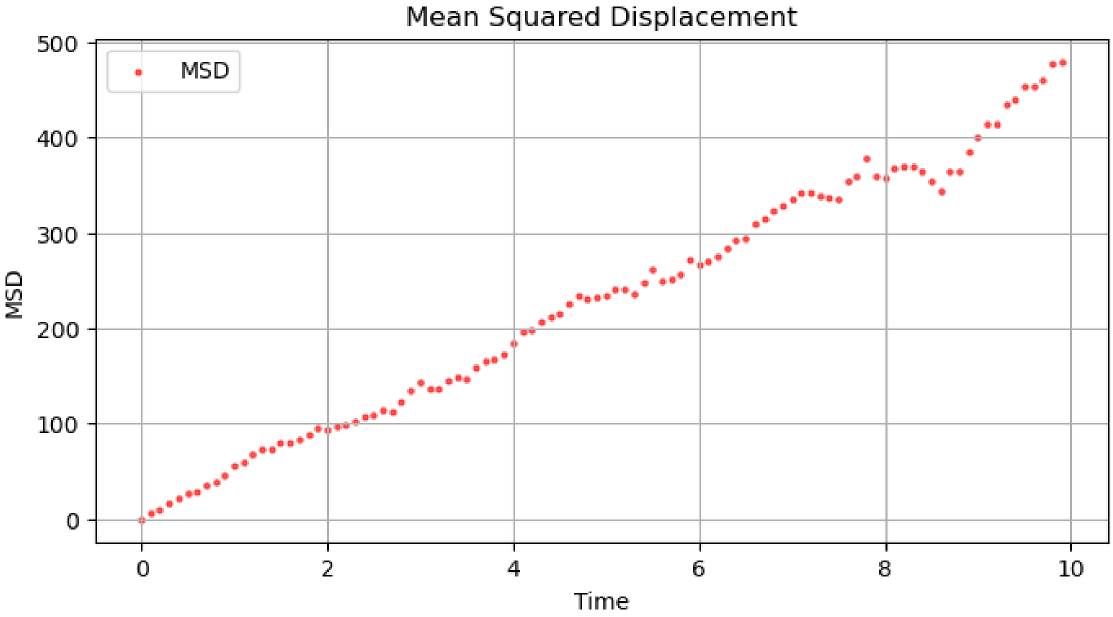
```
import numpy as np
import matplotlib.pyplot as plt

# Simulation parameters
time = 10
num_particles = 100
D = 24.0
dt = 0.1
num_steps = int(time / dt)

# Step size for Brownian motion
step_std = np.sqrt(2 * D * dt)

# Storage for particle positions
positions = np.zeros(num_particles)
trajectory = np.zeros((num_steps, num_particles))

# Simulate 1D Brownian motion
for t in range(num_steps):
    steps = np.random.normal(loc=0.0, scale=step_std, size=num_particles)
    positions += steps
    trajectory[t] = positions

# Plot a few sample trajectories
time_array = np.arange(num_steps) * dt
plt.figure(figsize=(8, 4))
for i in range(10):
    plt.plot(time_array, trajectory[:, i], linewidth=0.5)
    plt.scatter(0, trajectory[0, i], s=10)
    plt.scatter(time_array[-1], trajectory[-1, i], s=10)
plt.xlabel("Time")
plt.ylabel("Position (x)")
plt.grid(True)
plt.title("Sample 1D Brownian Trajectories")
plt.show()
```

Code 1: Simulation of 1D Diffusion



```
# Calculate MSD from trajectories
msd = np.mean((trajectory - trajectory[0])**2, axis=1)

# Plot raw MSD values
plt.figure(figsize=(8, 4))
plt.scatter(time_array, msd, s=5, color=’red’, alpha=0.6, label="MSD")
plt.xlabel("Time")
plt.ylabel("MSD")
plt.title("Mean Squared Displacement")
plt.grid(True)
plt.legend()
plt.show()
```

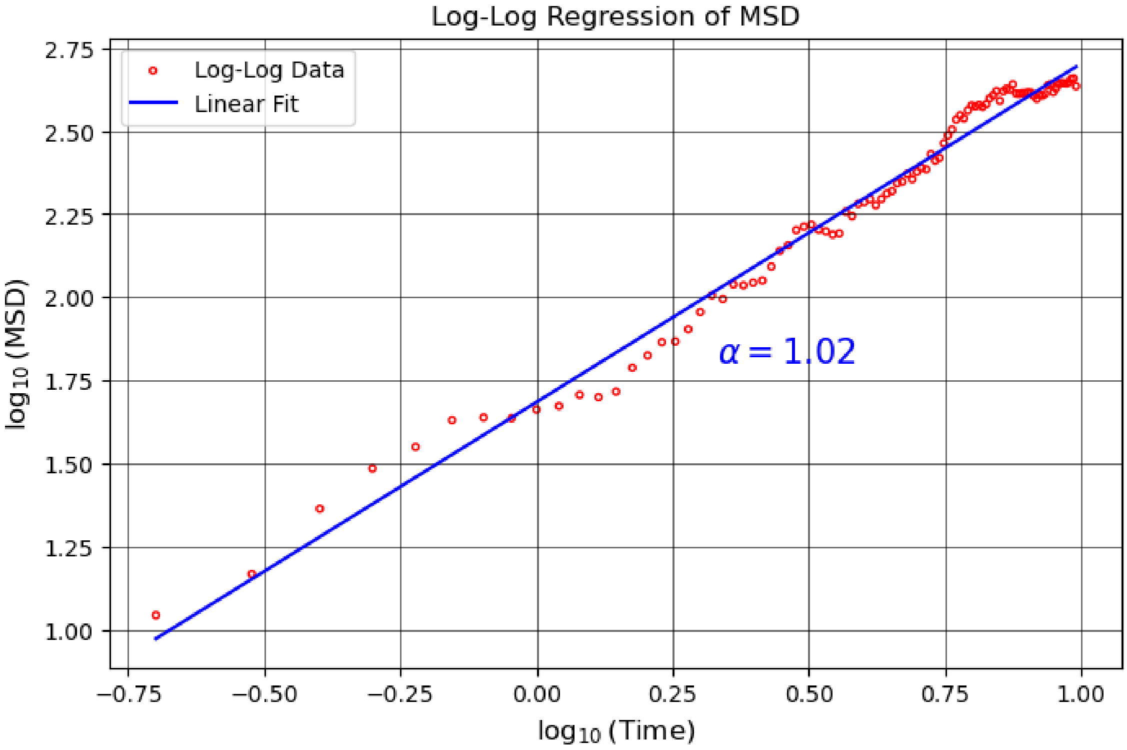
Code 2: Mean Squared Displacement


Mean Squared Displacement
MSD
MSD
500
400
300
200
100
0
0
2
4
6
8
10
Time

```python
from sklearn.linear_model import LinearRegression
import warnings

# Suppress divide-by-zero warning from log(0)
warnings.filterwarnings("ignore", message="divide by zero encountered in log")

# Prepare log-log data
valid = time_array > 0
log_time = np.log10(time_array[valid]).reshape(-1, 1)
log_msd = np.log10(msd[valid])

# Optional: slice fitting range
s = 1
e = -1
log_time_slice = log_time[s:e]
log_msd_slice = log_msd[s:e]

# Fit linear regression model in log-log space
model = LinearRegression()
model.fit(log_time_slice, log_msd_slice)

# Extract slope and intercept
slope = model.coef_[0]
intercept = model.intercept_
predicted_log_msd = model.predict(log_time_slice)

# Plot log-log MSD with linear regression
plt.figure(figsize=(8, 5))
plt.scatter(log_time_slice, log_msd_slice,
            edgecolors=’r’, facecolors=’none’, s=8, label=’Log-Log Data’)
plt.plot(log_time_slice, predicted_log_msd, color=’blue’, label=’Linear Fit’)

plt.text(0.6, 0.5,
         fr’$\alpha = {slope:.2f}$’,
         transform=plt.gca().transAxes,
         fontsize=15,
         weight=’bold’,
         color=’blue’,
         verticalalignment=’center’)

plt.xlabel(r’$\log_{10}$(Time)’, fontsize=12)
plt.ylabel(r’$\log_{10}$(MSD)’, fontsize=12)
plt.grid(True, which="both", linewidth=0.4, color=’black’)
plt.title("Log-Log Regression of MSD")
plt.legend()
```

```
plt.show()

# Print regression results
print("Log-Log Fit Results:")
print(f"  Slope (alpha)     = {slope:.4f} (expected ~1.0 for normal diffusion)")
print(f"  Intercept (log A) = {intercept:.4f}")
print(f"  Prefactor A       = {10**intercept:.4f}")
```

Code 3: Log-Log regression



2.2 Diffusion in 2D

Consider a particle moving in a two-dimensional space. Let $r(t)$ be the position of the particle at time t, given by

$$r(t) = (x(t), y(t)), \tag{2.9}$$

where $x(t)$ and $y(t)$ are the Cartesian coordinates at time t, each subject to its own diffusion process. The motion is governed by the SDE's

$$dx = \sqrt{2D}dB_x(t) \qquad\qquad dy = \sqrt{2D}dB_y(t), \tag{2.10}$$

where $B_x(t)$ and $B_y(t)$ are two independent Brownian motions. The displacement vector from the initial position $r_0 = (x_0, y_0)$ is given by

$$\overrightarrow{r}(t) - \overrightarrow{r_0} = (x(t) - x_0)\,\hat{\imath} + (y(t) - y_0)\,\hat{\jmath}. \tag{2.11}$$

Calculating the squared norm yields

$$\|\overrightarrow{r}(t) - \overrightarrow{r_0}\|^2 = (x(t) - x_0)^2 + (y(t) - y_0)^2. \tag{2.12}$$

Taking the expectation over all particle trajectories gives the MSD

$$\begin{aligned} \left\langle \|\overrightarrow{r}(t) - \overrightarrow{r_0}\|^2 \right\rangle &= \left\langle (x(t) - x_0)^2 + (y(t) - y_0)^2 \right\rangle \\ &= \left\langle (x(t) - x_0)^2 \right\rangle + \left\langle (y(t) - y_0)^2 \right\rangle \\ &= 2Dt + 2Dt \\ &= 4Dt. \end{aligned} \tag{2.13}$$

This result confirms that, in two dimensions, the MSD grows linearly with time t.

Simulation The following Python code simulates 2D Brownian motion for multiple particles and computes the MSD.

```
import numpy as np
import matplotlib.pyplot as plt

# Parameters
time = 1000       # Number of time steps
num_particles = 1000   # Number of particles
D = 24.0                # Diffusion coefficient
dt = 0.1               # Time step
num_steps = int(time / dt)  # Number of steps based on

# Standard deviation of step size based on Brownian motion
step_std = np.sqrt(2 * D * dt)

# Initialize positions
positions = np.zeros((num_particles, 2))  # Start at origin (0,0)
trajectory = np.zeros((num_steps, num_particles, 2))

# Simulate diffusion
for t in range(num_steps):
    steps = np.random.normal(loc=0.0, scale=step_std, size=(num_particles, 2))
    positions += steps
    trajectory[t] = positions

# Compute Mean Squared Displacement (MSD)
msd = np.mean(np.sum((trajectory - trajectory[0])**2, axis=2), axis=1)

# Plot sample trajectories
plt.figure(figsize=(8, 6))
num_to_plot = 1  # Number of particles to visualize
for i in range(num_to_plot):
    plt.plot(trajectory[:, i, 0], trajectory[:, i, 1], alpha=0.7, label=f"Particle {i+1}")
    plt.scatter(trajectory[0, i, 0], trajectory[0, i, 1], color='green', marker='o', s=50)  # Start point
    plt.scatter(trajectory[-1, i, 0], trajectory[-1, i, 1], color='red', marker='o', s=50)  # End point

#plt.title("Sample 2D Diffusion Trajectories with Start (green) and End (red)")
plt.xlabel("x")
plt.ylabel("y", rotation=0, labelpad=20)
plt.axis("equal")
plt.grid(True)
#plt.legend()
plt.show()

# Plot MSD vs Time
plt.figure(figsize=(8, 5))
plt.plot(np.arange(num_steps) * dt, msd)
```

```
#plt.title("Mean Squared Displacement (MSD) in 2D")
plt.xlabel("Time")
plt.ylabel("MSD")
plt.grid(True)
plt.show()
```

Code 4: Simulation of 2D Diffusion

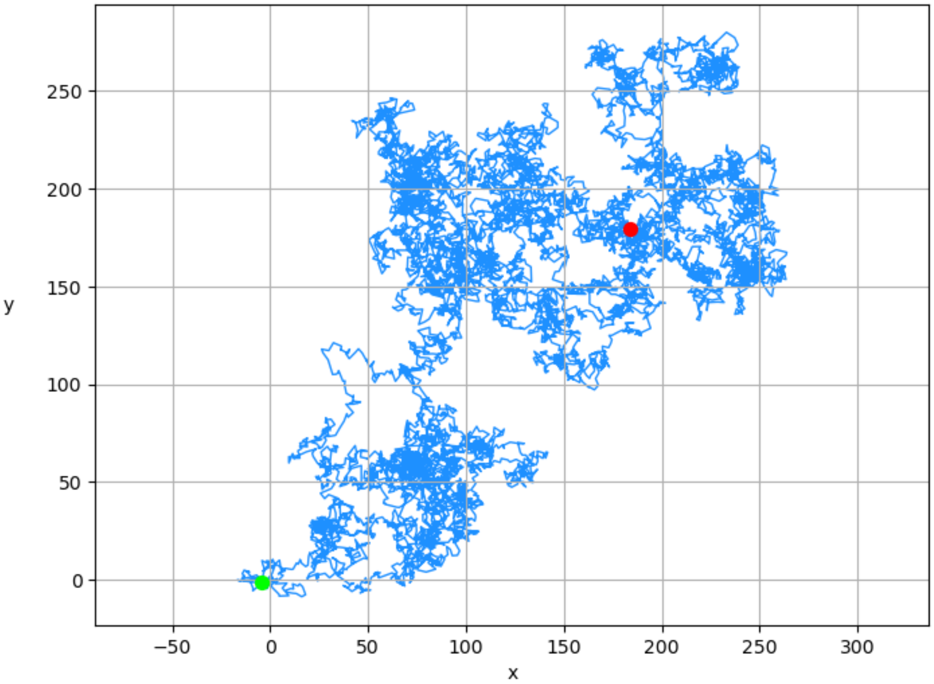


Figure 2.1:

2.3 Diffusion in d dimensions

In a general d-dimensional space, the position of a particle at time t is

$$r\left(t\right)=\left[x_1\left(t\right),...,x_d\left(t\right)\right], \tag{2.14}$$

where each coordinate $x_i\left(t\right)$ is subject to a diffusion process. The motion of each coordinate evolves independently and is governed by it own SDE fo the form

$$dx_i=\sqrt{2D}dB_i\left(t\right), \tag{2.15}$$

with $B_i\left(t\right)$ representing independent Brownian motions for each spatial direction $i=1,2,...,d$ and D being the diffusion coefficient. The displacement from the initial position can be described by the vector

$$\overrightarrow{r}\left(t\right)-\overrightarrow{r_0}=\left[x_1\left(t\right)-x_1\left(0\right),...,x_d\left(t\right)-x_d\left(0\right)\right]. \tag{2.16}$$

The squared norm is given by

$$\|\overrightarrow{r}\left(t\right)-\overrightarrow{r_0}\|^2=\sum_{i=1}^{d}\left[x_i\left(t\right)-x_i\left(0\right)\right]^2. \tag{2.17}$$

Taking the expectation over all trajectories yields the MSD

$$\begin{aligned}\left\langle\|\overrightarrow{r}\left(t\right)-\overrightarrow{r_0}\|^2\right\rangle &= \left\langle\sum_{i=1}^{d}\left[x_i\left(t\right)-x_i\left(0\right)\right]^2\right\rangle \\ &= \sum_{i=1}^{d}\left\langle\left[x_i\left(t\right)-x_i\left(0\right)\right]^2\right\rangle \\ &= \sum_{i=1}^{d}2Dt \\ &= 2dDt.\end{aligned} \tag{2.18}$$

Another way to present the relationship between MSD and time is

$$\left\langle\|r\left(t\right)-r_0\|^2\right\rangle\propto t, \tag{2.19}$$

which shows that, for simple diffusion process which undergo Brownian motion, the MSD grows linearly with time for large t.

3 Anomalous Diffusion

Anomalous diffusion is common in biological environments like cells, where obstacles and active transport processes lead to non-standard particle motion [4, 5]. When referring to the concept of anomalous diffusion, we mean that the MSD is not linear in time. Instead, the asymptotic behavior of the MSD scales with time as

$$\left\langle \| r\left(t\right) - r_0 \|^2 \right\rangle \propto t^{\gamma}, \tag{3.1}$$

where γ is a constant such that $\gamma \neq 1$. In the case where $\gamma = 1$ we come back to a normal diffusion process. There are several types of anomalous diffusion.

Sub-Diffusion This is a type of anomalous diffusion where particles spread out slower than expected based on normal diffusion models. In sub-diffusion, the MSD increases with time according to a power law where $0 < \gamma < 1$. In the context of biological systems such as cells, this type of diffusion is characterized by a non-linear relationship between the MSD and time. Specifically, for sub-diffusion, the MSD grows slower than linearly with time.

Super-Diffusion This is a type of anomalous diffusion where particles spread faster than they would under normal diffusion. The MSD scales as a power law where $1 < \gamma < 2$. Super-diffusion can occur in various physical systems and is often observed in complex systems where traditional Brownian motion does not adequately describe particle trajectories.

Ballistic Diffusion This is a type of anomalous diffusion which describes a physical phenomenon where particles move with constant velocity, leading to a MSD that scales quadratically with time, corresponding to $\gamma = 2$. In ballistic diffusion, particles exhibit straight-line motion without experiencing significant random scattering events typically observed in Brownian motion.

Hyper Ballistic Diffusion This type of anomalous diffusion represents an extreme form of particle motion, where the MSD increases faster than quadratically with time, corresponding to $\gamma > 2$. It is characterized by particles moving with continuously increasing velocity and persistent acceleration. In real physical systems, energy resources are finite, making such persistent acceleration impossible.

References

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