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Wandering in Uncertainty: Principles and Applications of Random Walks

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Abstract:

The phenomena of random walks are omniscient in nature. in this study, the author conducts an in-depth exploration of the properties of one, two, and three-dimensional random walks, emphasizing their interconnections. Through simulations of random walks across each dimension, the author carefully analyzes the displacement distribution and the mean squared displacement to classify the walks as either recurrent or transient. The results validate Pólya's Recurrence Theorem, demonstrating that random walks in one and two dimensions are recurrent, meaning that the walker has a high probability of returning to the origin. In contrast, random walks in three dimensions tend to be transient, where the walker is less likely to revisit the starting point. These findings are essential in the broader context of understanding Brownian motion, particularly in nanoconfined environments like DNA, where random motion significantly impacts molecular behavior. This study helps provide insights into how spatial constraints influence random movements at the nanoscale level.

Keywords: Random walk; Pólya's Recurrence Theorem; Brownian motion.

1. Introduction

This study will start to discuss the Pólya's Recurrence Theorem, developed by Hungarian mathematician George Pólya, and address the behavior of random walks in different dimensions. The theorem states that in one and two dimensions, a random walker is almost certain to eventually return to their starting point, making these walks "recurrent." This means that if given enough time, the walker will revisit the origin with probability 1 [1]. However, in three or more dimensions, the probability of returning to the starting point decreases as the dimensions increase, and the walk becomes "transient." In these cases, the walker may continue to move away from the origin indefinitely, with a lower likelihood of returning. Pólya's Recurrence Theorem has profound implications in fields like physics and biology, particularly in understanding phenomena like molecular diffusion and Brownian motion. After introducing the preconditions from the Pólya's Recurrence Theorem this study starts talking about motion at different dimensions in specific cases to determine each one's ability of returning [2]. Lastly, based on the above discussion, one can smoothly apply it to other disciplines such as Brownian motion in the biology field. The study will represent how do Markov chains play

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an essential role in biology.

Pólya's Recurrence Theorem is a significant conclusion of the study of random walks, particularly in the context of lattice-based random walks in different dimensions. The theorem provides idea that whether a random walker will eventually return to the starting point which is origin after an indefinite amount of time. Pólya's Recurrence Theorem states that, in one or two dimensions, a simple random walk on an infinite lattice is recurrent which means that the probability that the random walker will eventually return to the origin is 1 certainly [3]. On the other hand, in three or more dimensions, the random walk is transient which means that the probability that the random walker will eventually return to the origin is less than 1 and this non-zero probability refers that the walker will never return the start point.

The rest paper is organized as follows. In Sec. 2, the author will present the Pólya's Recurrence Theorem with details, and introduce the random walk in different dimensions. In Sec. 3, the author will introduce the application of Brownian motion. Finally, the last Section is devoted to the conclusion.

2. Methods and Theory

2.1 Pólya's Recurrence Theorem

According to the Polya's Recurrence Theorem, there is a theorem that the simple random walk on $\mathbb{Z}^d$ is recurrent in dimensions $d = 1,2$ and when $d \geqslant 3$ $\mathbb{Z}^d$ is transient. For instance, a walker has a probability of 1 of returning to origin since it moves in $\mathbb{Z}^2$. A runner, on the other hand, is less fortunate than a walker to return to its origin because it moves in $\mathbb{Z}^3$, meaning that the runner has a positive probability of never doing so [4].

Set a u_n a probability that a random walk is at 0 after n steps for $n \geqslant 0$. Notice that u_n=0 and at an even number of steps to be at 0 which means $u_1 = u_3 = u_5 = \ldots = 0$. Let f_n be the likelihood that a random walk will return to 0 for the first time at step n for $n \geqslant 1$, where is let $f_0 = 0$. Furthermore, let $f = \sum_{n=0}^{\infty} f_n$ then the probability of the random walk returning to 0 $= f$ and the probability of the random walk not returning to 0 which is reasonable equaled to $1 - f$ [5].

Breaking down each of the by taking into account the various times at which the random walk can first return to 0, or f_i, showing that $u_1 = f_0 u_1 + f_1 u_0$, $u_2 = f_0 u_2 + f_1 u_1 + f_2 u_0$, and

$$u_n = f_0 u_n + f_1 u_{n-1} + \ldots + f_n u_0 \#(1)$$

for arbitrary n. Each decomposition is modeled by $f_0 u_{n-k}$, where the random walk first retuens returns after k steps and then in $n-k$ steps backs to 0, and the qualities can be obtained by repeating the above argument.

Let $U(s) = u_0 + u_1 s + u_2 s^2 + \cdots$ and $F(s) = f_0 + f_1 s + f_2 s^2 + \cdots$, then, $U(s)F(s) = u_0 f_0 + (f_0 u_1 + f_1 u_0)s + (f_0 u_2 + f_1 u_1 + f_2 u_0)s^2 + \ldots = U(s) - 1$, meaning that $1 = U(s)(1 - F(s))$. Identifying the requirements for transition and recurrence,

If $\sum_{n=0}^{\infty} u_n = \infty$, then $f = 1$ refers that the random walk is recurrent. On the other hand, If $\sum_{n=0}^{\infty} u_n < \infty$, then $f < 1$ refers to the transient random walk.

To prove this criterion, $\sum_{n=0}^{\infty} u_n = \infty$ means that

$$\lim_{s\to1} U(s) = \infty, \text{ so } \lim_{s\to1} 1 - F(s) = \lim_{s\to1} \frac{1}{U(s)} = 0, \lim_{s\to1} F(s) = 1$$

which indicate that $f = 1$ means the random walk is recurrent. In the end, $\sum_{n=0}^{\infty} u_n < \infty$ means that $\lim_{s\to1} U(s) < \infty$ so $\lim_{s\to1} 1 - F(s) = \lim_{s\to1} \frac{1}{U(s)} > 0$ infers $\lim_{s\to1} F(s) < 1 (f < 1)$ means the random walk is transient.

2.2 The Cases of Random Walk

The random walk model's basic idea is to traverse a graph beginning at one or more vertices. The walker has two probabilities at any given vertex in the graph: 1-P for moving to a neighboring vertex and P for randomly teleporting to any vertex. P is called the teleportation probability. Following every stroll, a probability distribution is produced, signifying the possibility of seeing every vertex within the graph. The next walk then uses this probability distribution as its input, and the cycle continues in this manner. This probability distribution will converge under specific circumstances, producing a stable distribution. Once convergence is achieved, a stable probability distribution is obtained.

2.2.1 The Case of One Dimension

Firstly, in the case of one dimension, if

$\sum_{i=1}^{\infty} f_i = 1 \Leftrightarrow \sum_{n=1}^{\infty} u_n = 0$, then $\sum_{n=1}^{n} u_{2n} = \infty$. The total steps of the entire walk is [6]

$$u_{2n} = \binom{2n}{n} = \frac{2n!}{n!n!}\left(\frac{1}{2}\right)^{2n} \quad (2)$$

To calculate u_{2n}, using the Stirling approximation to n!, $n!\sqrt{2\pi n}\left(\frac{n}{e}\right)^n$ and changing u_{2n} into that $u_{2n} = \frac{\binom{2n}{n}}{2^{2n}}$, $\binom{2n}{n} = \frac{(2n)!}{n!n!} \cong \frac{\sqrt{2\pi 2n}\left(\frac{2n}{n}\right)^{2n}}{\left(\sqrt{2\pi n}\left(\frac{n}{2}\right)^n\right)^2}$

$= \frac{e^{-2n}\cdot\sqrt{2}\cdot\sqrt{2\pi n}\,(2)^{2n}(n)^{2n}}{e^{-2n}\cdot\left(\sqrt{2\pi n}\right)^2 (n)^{2n}} = \frac{2^{2n}}{\sqrt{\pi n}}$. Therefore, u_{2n} is represented that $u_{2n} = \frac{\binom{2n}{n}}{2^{2n}} \cong \frac{\frac{2^{2n}}{\sqrt{\pi n}}}{2^{2n}} = \frac{1}{\sqrt{\pi n}}$. To determine whether the random walk in one dimension is recurrent or transient, deciding $U(1)$ is divergent or convergent so showing that $U(1) = \sum_{n=0}^{\infty} u_{2n} \cong \frac{1}{\sqrt{\pi}}\sum_{n=0}^{\infty}\frac{1}{n^{\frac{1}{2}}} = \infty$ which represents the convergence. Thus, for one dimension, $P(u_{2n}=0) = F(1) = 1-\frac{1}{\infty} = 1$ which means it is recurrent.

2.2.2 The Case of Two Dimensions

Secondly, in the case of two dimension, according to the Polya's Recurrence Theorem, known that if n is even the nth step probability is 0. In two dimensions, there is four different directions and without any bias the probability of each direction is the same which is $u_{2n} = \left(\frac{1}{4}\right)^{2n}$. The number of return paths equals to $\frac{(2n)!}{x!x!(n-x)!(n-x)!}$ so the total number of return paths equals to $\sum_{x=0}^{n}\frac{(2n)!}{x!x!(n-x)!(n-x)!}$.

To calculate the paths, it follows that

$$P_{2nthstepreturn} = \left(\frac{1}{4}\right)^{2n}\sum_{x=0}^{n}\frac{(2n)!}{x!x!(n-x)!(n-x)!}\bullet\frac{1}{n!} \quad (3)$$

and simplifying this equation into

$P = \left(\frac{1}{4}\right)^{2n}\sum_{x=0}^{n}\frac{n!}{x!(n-x)!}\bullet\frac{n!}{x!(n-x)!}\bullet\frac{(2n)!}{n!n!}$ further simplification is that $\mathrm{P} = \left(\frac{1}{4}\right)^{2\mathrm{n}}\binom{2\mathrm{n}}{\mathrm{n}}\sum_{\mathrm{x}=0}^{\mathrm{n}}\left(\binom{\mathrm{n}}{\mathrm{x}}\right)^2$ [7]. After sorting the initial one, the final equation is $\mathrm{P} = \left(\binom{2\mathrm{n}}{\mathrm{n}}\frac{2}{2^{2\mathrm{n}}}\right)^2$ which is equaled to $(u_{2n})^2$. Also, $u_{2n}\,\mathbb{C}\frac{1}{\left(n^{\frac{1}{2}}\right)^2} = \mathbb{C}\frac{1}{n}$ and notice, the $\mathbb{C}\frac{1}{n}$ here because the power of n is 1 it is divergent. There is a formula could be worked here is that

$$(a+b)^n = a^n + \binom{n}{1}a^{n-2}b^2 + \ldots + \binom{n}{r}a^{n-r}b^r + \ldots + b^n \quad (4)$$

for $n\in\mathbb{N}$ where $\binom{n}{r} = \frac{n!}{r!(n-r)!}$ which could lead $\sum_{x=0}^{n}\left(\binom{n}{x}\right)^2 = \binom{2n}{n}$.

Because $(1+x)^{2n}$ the left hand could be written into that $(1+x)^n(1+x)^n$ which equals to $\left(\mathbb{C}_n^0 1^0 x^n + \mathbb{C}_n^1 1^1 x^{n-1} + \ldots + \mathbb{C}_n^{n-1}1^{n-1}x^1 + \mathbb{C}_n^n 1^n x^0\right)^2$ both have the same power 2 the initial one $(1+n)^{2n}$ equals to $\mathbb{C}_{2n}^0 1^0 x^{2n} + \mathbb{C}_{2n}^1 1^1 x^{2n-1} + \ldots + \mathbb{C}_{2n}^{2n-1}1^{2n-1}x^1 + \mathbb{C}_{2n}^{2n}1^{2n}x^0$. Furthermore, according to $\mathbb{C}_{2n}^n 1^n x^n = \mathbb{C}_{2n}^n x^n$, for two dimensions, $P\left(u_{2n} = \frac{\mathbb{C}}{n}\right), \sum_{n=0}^{\infty}\frac{1}{n} = \infty$, $1-\frac{1}{\infty} = 1$ which means it is recurrent.

2.2.3 The Case of Three Dimensions

Thirdly, in the case of three dimension there is six different directions could be walked to so the number of walks that come back to the origin in 2n steps is $\left(\frac{1}{6}\right)^{2n}$ because there is no bias that determine which direction will go to. Let k represents the steps left or up into the board and j represents the right or down out of the board, j is the number of steps in (1,0,0) direction, k is the number of steps in (0,1,0) direction. Therefore, there are the preconditions that $0\leqslant j$, $0\leqslant k, k+j\leqslant n$ and $2k+2j+2(n-k-j) = 2n$ which there are $n-j-k$ steps walking in the direction $(0,0,1)$. The number of walks that return to the origin

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in 2n steps is $u_{2n}=6^{-2n}\sum_{\substack{j,k\geqslant 0,\\ j+k\leqslant n}}\frac{(2n)!}{\left(j!k!(n-j-k)!\right)^2}$. By sorting this equation getting that

$$u_{2n}=6^{-2n}\binom{2n}{n}\sum_{\substack{j,k\geqslant 0\\ j+k\leqslant n}}\left(\frac{n!}{j!k!(n-j-k)!}\right)^2 \quad (5)$$

dividing 6 into 2×3 and changing the position of 3,

$$u_{2n}=2^{-2n}\binom{2n}{n}\sum_{\substack{j,k\geqslant 0,\\ j+k\leqslant n}}\left(3^{-n}\frac{n!}{j!k!(n-j-k)}\right)^2,$$

where there are 3^n such n letter strings, from

$$\sum_{\substack{j,k\geqslant 0\\ j+k\leqslant n}}3^{-n}\frac{n!}{j!k!(n-j-k)!}=1.$$

Continuously, it is possible to show that

$$\sum_{\substack{j,k\geqslant 0\\ j+k\leqslant n}}\left(3^{-n}\frac{n!}{j!k!(n-j-k)!}\right)^2\leqslant max\left(3^{-n}\frac{n!}{j!k!(n-j-k)!}\right)$$

, from which it follows that

$u_{2n}\leqslant 2^{-2n}\binom{2n}{n}\max\left(3^{-n}\frac{n!}{j!k!(n-j-k)!}\right)$. To solve this equation, using Stirling's formula again, it is found that

$$\frac{n!}{j!k!(n-j-k)!}\frac{\sqrt{2\pi n}\left(\frac{n}{e}\right)^n}{\sqrt{2\pi n}\left(\frac{j}{e}\right)^j\sqrt{2\pi n}\left(\frac{k}{e}\right)^k\sqrt{2\pi(n-j-k)}\left(\frac{n-j-k}{e}\right)^{n-j-k}}=\frac{\sqrt{n}}{\sqrt{j!k!(n-j-k)!}}\frac{n^n}{j^jk^k(n-j-k)^{n-j-k}}.$$

It is the standard analytical exercise to determine that j and k are equal as well as $n-j-k\approx\frac{n}{3}$, maximizing the value from above equation.

Assuming that $\frac{n}{3}$ is integer for ease of computation. All

$$max\left(3^{-n}\frac{n!}{j!k!(n-j-k)!}\right)=$$

in all, $3^{-n}\bullet\frac{\sqrt{n}}{\sqrt{\frac{n}{3}\bullet\frac{n}{3}\bullet\frac{n}{3}}}\bullet\frac{n^n}{\left(\frac{n}{3}\right)^{\frac{n}{3}}\left(\frac{n}{3}\right)^{\frac{n}{3}}\left(\frac{n}{3}\right)^{\frac{n}{3}}}=3^{-n}\bullet\frac{C}{n}\bullet 3^n=\frac{C}{n}$

where c is probably $3\sqrt{3}$. However, constant likely the purpose so $u_{2n}\leqslant 2^{-2n}$ (\genfrac0 pt2nn) $\bullet\frac{C}{n}\frac{1}{\sqrt{\pi n}}\bullet\frac{C}{n}=\frac{C}{n^{\frac{3}{2}}}$

which is also meaning that $\sum_{n=0}^{\infty}u_{2n}=\sum_{n=0}^{\infty}\frac{C}{n^{\frac{3}{2}}}<\infty$, indicating the divergence meaning that it is transient.

3. Brownian Motion and its Applications

3.1 Brownian Motion

Named for the botanist Robert Brown, who in 1827 made the first observation of the erratic movement of pollen grains suspended in water, Brownian motion is a basic idea in probability theory and stochastic processes. In a random walk, a particle takes steps in random directions at discrete time intervals. Each step is independent of the previous ones, and the overall position of the particle after many steps is determined by the cumulative effect of these random steps. Similarly, Brownian motion, also known as a Wiener process, models the movement of particles suspended in a fluid, where the particle's path is continuous and has continuous derivatives. Also, there are no jumps or discontinues in the path of the process. Then, the properties are characterized.

Firstly, the changes in position over non-overlapping time intervals are independent of each other. In other words, the position change from time t to $t+s$ is independent of the position change from time $t'+s'$, provided that the intervals do not overlap. Secondly, the change in position over any time interval Δt follow a normal distribution with mean zero and variance proportional to Δt. Specifically, if $X(t)$ denotes the position at time t, then $X(t+\Delta t)-X(t)N(0,\sigma^2\Delta t)$, where σ^2 is the variance parameter. Thirdly, the distribution of the increment over any given time interval is independent of the beginning point and solely dependent on the interval's length. Finally, the length of the interval—rather than the starting point—is the only factor that affects how the increment is distributed over any given time period. Formally, a Brownian motion $\{W(t),t\geqslant 0\}$ could be defined as a stochastic process satisfying: $W(0)=0$, $W(t)-W(s)N(0,t-s)$ for $0\leqslant s<t$.

3.2 Application

The Brownian Motion could be used to support a discussion that Conclusion- Dissecting the power spectral density of the z position (S_z) using a numerical approach based on Kramers equations.

TA Brownian particle moving over a long period of time (diffusive motion) can also be described by the Kramers equation in the short term (inertial motion). IIt is assumed and physically expected that the probability density function will vanish at infinite distances from the source if people consider infinite geometries. However, if people take finite geometry into account, the circumstances may differ. However, points of interest in the present study (e.g., the understanding of S_z) have not been addressed previously. Considering that a free particle in an arbitrary potential V(z) and has been applied to obtain the presence probability as S_z from the FFT of the auto-correlation function (in the following Fig. 1) [8]. The dimensionless units used in the simulations are:

- Time t/t_{unit} can be chosen arbitrarily
- Thermal velocity $V_{th} = (k_b T/m)^{0.5}$ (from the kinetic energy ½m $V_{th}^{0.5}$ = ½ k_b T)
- Velocity $V \leftrightarrow v = V/\left(V_{thT_{unit}}\right)$
- Momentum $P = mV \leftrightarrow p = p/(mV_{th}) = v$
- Spring constant $Kc \leftrightarrow kc = K_c / mt_{unit}^2 = \Omega_0^2 = \omega 0^2$
- Potential $U(z) \leftrightarrow u(x) = U(z)/(k_b T)$
- Harmonic potential $½ K_c Z^2 \leftrightarrow ½ kcz^2$
- Angular frequency $\Omega_0 = (K/m)^{0.5} \leftrightarrow \omega_0 = \Omega t_{unit}$
- Diffusion constant $D = (k_b T)/(mg) = V_{th}^2/\Gamma_0 \leftrightarrow d = D/\left(V_{th}^2\right) = 1/g$.
- Overdamp: $\Gamma_0 > 2\omega_0$; underdamped $\Gamma_0 < 2\omega_0$; $\Gamma_0 = 1/2Q$.

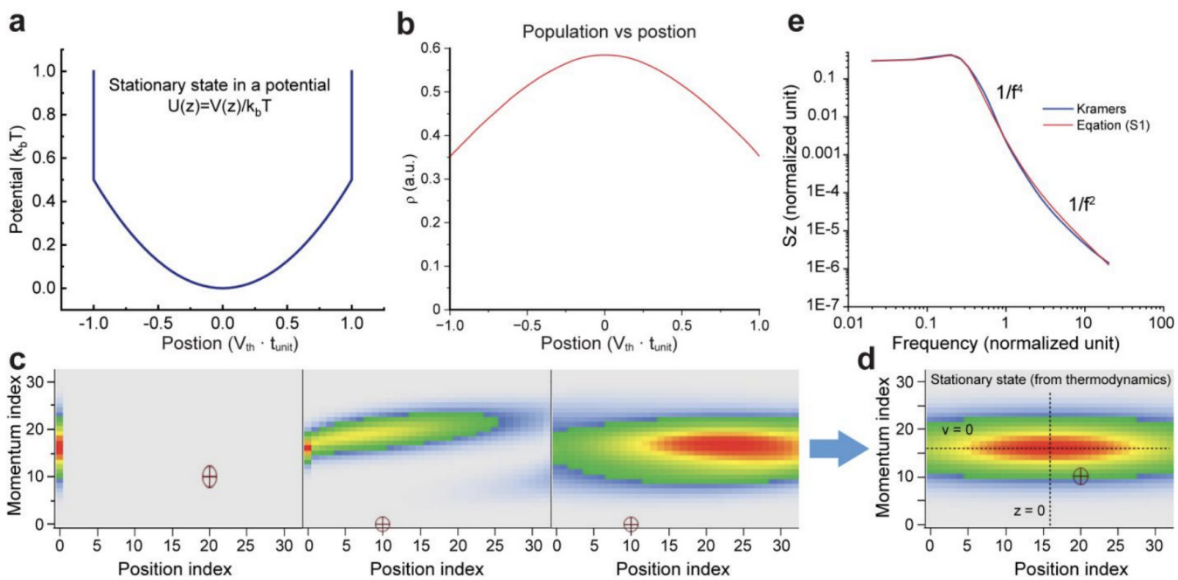

Fig.1 The key aspects of the system under study [8].

Figure 1 presents several key aspects of the system under study. In (a), the potential shape is depicted as a combination of a harmonic potential, represented by $V(z)$, with reflective boundaries added to simulate the effects of confining walls. In (b), the simulated probability distribution shows the likelihood of a particle being present within this potential. Panel (c) illustrates an example of how the probability distribution $P(z, p, t)$ evolves over time in phase space. In (d), one can see the system's stationary state, where the dynamics settle into a stable configuration in phase space. Finally, panel (e) shows the power spectral density (PSD) for the system, calculated using the Fast Fourier Transform (FFT) of the auto-correlation function. The PSD is compared in both the presence and absence of confinement to highlight the system's response under different conditions.

Parameters used were $g = 0.5(Q = 1)$, k_c = 1, l_z = 2. The simulation does confirm that the consideration of reflective boundary conditions includes a resonance, $1/f^4$ dependence, and a $1/f^2$ dependence at high frequency (black curve in Fig. 1(e)). A semi-empirical equation can be used to reproduce Brownian motion spectra with reflective boundaries. It assumes the superposition of two equal contributions. One is that the author neglects boundary condi-

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tions, while the other is that a diffusive Brownian particle with reflective walls that leads to a Lorentzian spectrum with $1/f^2$ dependence at high frequency.

The derivation of the first term is obtained starting from a stochastic two-level system. For simplicity, the author assumes a single frequency $D/z_{gap}{}^2$, which can be assumed as the Kramers frequency f_k that differs only by a factor π/2 if one considers Einstein's relation $\gamma^D = \beta^{-1}$. Finally, it is found that

$$S_z = 0.5\frac{4D/2\pi}{\left[f_k^2 + f^2\right]} + 0.5\frac{2}{\beta k_c f_0}\frac{1/Q}{\left[\left[1-\left(\frac{f}{f_0}\right)^2\right]^2 + \left[\frac{f}{f_k}\right]^2\right]} \quad (6)$$

where D is chosen to fit PSD from OxDNA simulations is very close to the diffusion coefficient for one bead in the coarse-grained model $\left(0.7\times10^9 nm^2 s^{-1}\right)$ [8].

4. Conclusion

In conclusion, this study has conducted a thorough analysis of random walks and their applications within the realm of biology particularly in understanding molecular processes. By investigating the core principles and mathematical models underlying random walks the author has highlighted their unique property of returning to the origin. This phenomenon is crucial in various fields, including the study of diffusion and molecular motion. The simulation results further reinforce the theoretical predictions, showcasing how random walks play a significant role in understanding ballistic Brownian motion, especially in nanoconfined DNA. The ability of random walks to explain the trajectory and movement of particles within confined spaces provides valuable insights into the behavior of bio-molecules under such conditions. Nanoconfined DNA is particularly relevant here as it exhibits unique motion characteristics when constrained and random walk models help to elucidate these behaviors. Furthermore, the study confirms the relationship between the number of steps in a random walk and the mean squared displacement, which is linearly proportional. This consistency with theoretical predictions further validates the robustness of random walks as a model for molecular motion. The implications of this work extend beyond theoretical understanding which helps understand particle movement at the nanoscale is essential.

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