

THERMAL MOTION OF SMALL PARTICLES

DIFFUSION

Martin Jasinski

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Yes Yes !!!.

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INTRODUCTION

- Why is diffusion interesting...
- what are the key global principles?

The physical processes of the world around us act very strangely in the regime of the nano-world. Some notable differences are the scale of electrostatic forces, drag forces of different media, and thermal effects. Of the three mentioned, thermal effects are a driving force of motion. From an energetic perspective, the equipartition theorem states that for each degree of freedom the kinetic energy applied is given by:

$$E_{\text{kin}} = \frac{3}{2} k_B T \quad (1)$$

In a world where there are no frictional losses and all energy is transformed into kinetic energy, the average speed of a particle is then scaled according to:

$$|v_i|^2 = \frac{k_B T}{m} \quad (2)$$

where i denotes the basis of the vector direction, k_b is the Boltzmann constant, and T is temperature. This intermediate result shows that as $k_B T \propto m$ the mean square velocity is clearly non-zero. This in turn results in a net displacement, or a **Diffusive Process**.

This energetic reality motivates the need to study processes that describe the microscopic movement of particles in more realistic systems including the aforementioned contributions. In addition, a general framework of such processes should be of interest, that of which includes not only fluid contributions, electromagnetic, but also to an extent quantum effects.

The relevant systems which this applies to can be found in various fields such as biological physics, chemical engineering, heat processes and many others.

CHAPTER 1

1.1. DIFFUSION FROM MASS CONSERVATION

To begin discussion about diffusion, it is necessary to derive it from basic physical origins.

The particles in a solution can be defined in terms of a commonly measurable quantity: concentration. The concentration of a fluid can be measured by terms of mass per volume, or $\frac{g}{ml}$ for instance.

Thus, the flow of concentration can be modeled via the physical law of mass conservation. Specifically, since the flux at the boundaries of a tube is equation to the change in the concentration in the volume, the law takes on the following form:

$$V \frac{\partial c(x, t)}{\partial t} = A_{\text{in}} Q(x + \Delta x, t) - A_{\text{out}} Q(x, t) \quad (1.1)$$

Where V is the volume, A is the cross-sectional area of the flow. As we can note, the units that both sides of the equation hold are units of mass. Thus, by expanding the volume in terms of cross-sectional area times an infinitely small displacement Δx , $V = A\Delta x$. Note that this forces both areas to be identical in the limit of $\Delta x \rightarrow 0$.

$$\frac{\partial c(x, t)}{\partial t} = \frac{Q(x + \Delta x, t) - Q(x, t)}{\Delta x} \quad (1.2)$$

Then, by taking the limit:

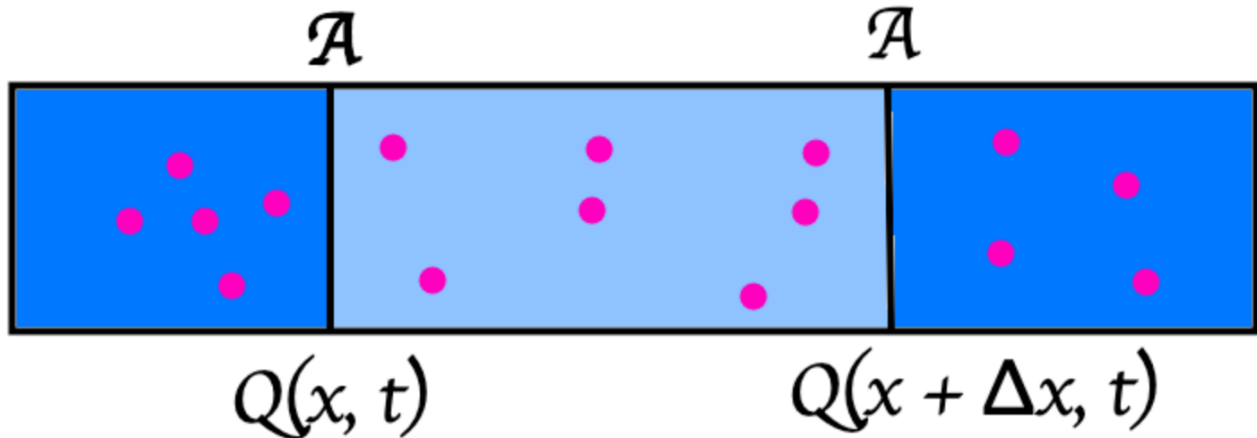
$$\frac{\partial c(x, t)}{\partial t} = \frac{\partial Q(x, t)}{\partial x} \quad (1.3)$$

Then, noting that the unitary relationship between the concentration and the flux is a spatial term in the denominator. However, this is ad hoc. Rigorous treatment of this is difficult as it relies on the principle of a relationship between concentration of particles and flux through a surface. This is simply stated as $Q = -D \frac{\partial c}{\partial x}$. Thus, we arrive at the one-dimensional diffusion equation.

$$\frac{\partial c(x, t)}{\partial t} = D \frac{\partial^2 c(x, t)}{\partial x^2} \quad (1.4)$$

This result is expected from the treatment of particles as fluids. Curious readers may recall this is the form of the heat equation, which holds the same principle of conserved mass. As in the heat equation, the three dimensional case of this equation naturally extends via the Laplace operator. This will later be formulated in anisotropic diffusion, however, for now, the big picture of diffusion is then given by the following equation:

$$\frac{\partial c(\vec{r}, t)}{\partial t} = D \nabla^2 c(\vec{r}, t) \quad (1.5)$$



1.2. SOLUTIONS OF THE DIFFERENTIAL MODEL

Given the powerful model of diffusion derived, there are important physical quantities which should be uncovered, right? First, lets solve the diffusion equation and interpret the results. For simplicity, we will return to the 1-dimensional case, which should describe the physical principles in a digestible way.

To solve the linear 2nd order PDE, the solutions can be easily derived as found in appendix A.

1.3. CONCLUSIONS

The differential formulation of diffusion provides insight to the bulk behavior of molecules on the macro scale. In the context of large-scale systems, such as particle dispersion, heat diffusion, or other similar processes, this describes the time-dependent equations on which the process evolves. In the large-scale, ergodic limit, all possible states are highly likely to be filled given the assumption all particles are equal. Further discussions in this regime fall under details of materials and diffusion tensors, which are applicable in the context of medical imaging, engineering, and other applied sciences. The discussion of the diffusion tensor is left to the appendix as it is pretty cool, but not relevant to my studies.

CHAPTER 2

The single molecule approach to diffusion is a very intuitive picture of how microscopic things move. This formulation emphasizes itself on how the motion of a single particle causes the macroscopic properties of diffusion, as deduced by the macroscopic picture, to naturally arises, proving themselves.

The discussion of non-equilibrium diffusion is a discussion about Brownian motion, or the random movement of particle in a thermal bath. Recalling some basic properties from equilibrium statistical mechanics, the possible states of a particle can be described by the Hamiltonian. This formulation assumes no losses and other annoying effects, however, it paints a picture for how to treat Brownian motion. In a potential, a simple, ideal particle will have the partition function given by the following sum:

$$Z = \sum_{\{i\}} \exp[-\beta(\mathcal{H})] \quad (2.1)$$

Where $\mathcal{H} = \frac{1}{2}m_i\dot{x}^2 + V(x, \dot{x})$. The sum $\{i\}$ denotes the sum over all possible states. What this fundamental equation describes is that the number of combination scales with the total energy in the system. Given a unique, or complicated potential, the total set of particles and some influx, or Canonical exchange of energy, such as a heat bath, there will be a set of possible energy states which the particle will take on.

So, a Brownian particle is placed into a heat bath, what now? Given that the particle will undergo thermodynamic heat transfer, the particle will gain energy. Due to the consequences of the equipartition theorem, we can deduce that the thermal energy will couple with the kinetic properties of the particle.

$$\begin{aligned} T &= \frac{1}{2}m\dot{x}^2 = \frac{1}{2}k_bT \\ \rightarrow \dot{x} &= \sqrt{mk_bT} \end{aligned} \quad (2.2)$$

This energetic result causes the particles to move in a violent, stochastic manner. This property is the sole cause of Brownian motion.

2.1. LANGEVIN EQUATIONS

To start the journey into this beautiful realm of mathematics, Newton's law (of course!) is enacted. To be accurate, we must account for a simple particle in empty space. There is no resistances, that is, there is no friction. In the case of a thermal bath, such as that of a non-reactive, ideal gas the contributions to the forces of the particle will be stochastic in direction. This stochastic force is a stochastic process¹ which describes the vector addition of forces to the particle.

The properties of this stochastic force have great significance. As a start, lets assume a simple process where there is a large heat reservoir which places a uniformly random direction and constant intensity impulse each time step. Denote this random variable $\vec{\eta}(t)$. Newton's law then reads:

$$m\ddot{\vec{x}} = \vec{\eta}(t) \quad (2.3)$$

To obtain the equation of motion from this equation, we can simply take integrals over time.

$$\vec{x}(t) = x_0 + tx_1 + \frac{1}{m} \int_0^t \int_0^{t'} \vec{\eta}(t) dt dt' \quad (2.4)$$

Sadly, unless we know the exact trace of $\vec{\eta}$, this is incalculable. Instead, we can take a more natural quantity, the average and variance. In addition, working with position is difficult due to the coordinate system in place. in 3

¹See Appendix for more details on this topic.

dimensions, the free movement of such a particle is non-holonomic in the sense that unless each step is kept track of, the overall position of the particle cannot be determined. Thus, in this formulation, it is easier to discuss the velocity of the particle.²

The velocity of the particle is then described as:

$$\begin{aligned}\dot{\vec{v}} &= \frac{1}{m}\vec{\eta}(t) \\ \rightarrow \vec{v} &= \frac{1}{m} \int_0^t \vec{\eta}(t') dt'\end{aligned}\tag{2.5}$$

The average can be computed by averaging over all possible realizations (states) of η .

$$\langle \vec{v} \rangle = v_0 + \frac{1}{m} \int_0^t \langle \vec{\eta}(t') \rangle dt' \tag{2.6}$$

Since the average is uniform in all directions, the total average is 0, which states that in the long-term, the particles net velocity is constant, equal to v_0 .

This is perfectly valid, as the velocity is a stationary random process, which states that the average velocity of the particle does not depend on time. However, this poses a problem. The average position can be calculated.

$$\langle \vec{x} \rangle = \vec{v}_0 t + \vec{x}_0 \tag{2.7}$$

This however, is deeply unphysical. I don't see particle moving infinitely due to a small initial velocity. The key detail in this formulation is a velocity dependent damping force³. The Langevin equation factors in a linear velocity term, which produces the fundamental equation for Langevin Brownian motion.

$$m\dot{\vec{v}} = -\lambda\vec{v} + \vec{\eta}(t) \tag{2.8}$$

The solution to this equation can be solved analytically. The solution is split into the homogenous and particular solution, which are both analytically solvable. The homogenous solution entails solving:

$$\begin{aligned}m\dot{\vec{v}} + \lambda\vec{v} &= 0 \\ \rightarrow v &= v_0 \exp\left[-\frac{\lambda}{m}(t - t_0)\right]\end{aligned}\tag{2.9}$$

The particular solution can be solved by applying an integration factor of $e^{\frac{\lambda}{m}(t-t_0)}$. The Langevin equation becomes:

$$\frac{d}{dt} \left(v \exp \left[\frac{\lambda}{m}(t - t_0) \right] \right) = \eta(t) \exp \left[\frac{\lambda}{m}(t - t_0) \right] \tag{2.10}$$

²A quick aside, the positional average and variance can be calculated simple given some constraints. For instance, if the particle was confined to a lattice, then the problem becomes a combinatorial problem which can be solved. For more information, see [?]

³This isn't really well explained even in the literature. Intuitively, such this is okay, but I'm not sure how to physically 'prove' this is necessary

SOLUTIONS TO THE DIFFUSION EQUATION

A.1. 1D FREE DIFFUSION EQUATION VIA FOURIER TRANSFORM

The boundaries of the problem are stated that at very large x , the concentration is equation to 0. The easiest way to solve this equation is to use the Fourier transform. This is mainly due to the boundary conditions of this problem.

The diffusion problem starts with the equation of diffusion:

$$\partial_t c(x, t) = D \partial_{xx} c(x, t) \quad (\text{A.1})$$

Take the Fourier transform of both sides. We can denote the Fourier transform as a hat $\widehat{c(x, t)}$.

$$\int_{-\infty}^{\infty} \partial_t c(x, t) \mathbf{exp}[-ikx] dx = \int_{-\infty}^{\infty} D \partial_{xx} c(x, t) \mathbf{exp}[-ikx] dx \quad (\text{A.2})$$

The LHS of this equation is trivial due to Fubini's theorem.

$$\int_{-\infty}^{\infty} \partial_t c(x, t) \mathbf{exp}[-ikx] dx = \partial_t \widehat{c(x, t)} \quad (\text{A.3})$$

The RHS can be simplified using an integration by parts.

$$\begin{aligned} \int_{-\infty}^{\infty} \partial_{xx} c(x, t) \mathbf{exp}[-ikx] dx &= \int_{-\infty}^{\infty} \partial_x c(x, t) \mathbf{exp}[-ikx] (-ik) dx \\ &= \int_{-\infty}^{\infty} c(x, t) \mathbf{exp}[-ikx] (ik)^2 dx \\ &\rightarrow (ik)^2 \widehat{c(x, t)} \end{aligned} \quad (\text{A.4})$$

The full equation then reads:

$$\begin{aligned} \partial_t \hat{c}(k, t) &= D(ik)^2 \hat{c}(k, t) \\ \partial_t \hat{c}(k, t) + Dk^2 \hat{c}(k, t) &= 0 \end{aligned} \quad (\text{A.5})$$

Using an integration factor $\mathbf{exp} \left[\int Dk^2 dt \right]$:

$$\partial_t [\hat{c}(x, t) \mathbf{exp} [Dk^2 t]] = 0 \quad (\text{A.6})$$

This can then be solved using a simple integration with respect to t . This gives the arbitrary constant some random dependence on k .

$$\hat{c}(x, t) = f(k) \mathbf{exp} [-Dk^2 t] \quad (\text{A.7})$$

The full solution is then given using the inverse Fourier transform.

$$c(x, t) = \int_{-\infty}^{\infty} f(k) \mathbf{exp} [-Dk^2 t] \mathbf{exp} [ikx] dk \quad (\text{A.8})$$

This is the solution in disguise. Since the initial condition implies that $c(x, 0) = f(x)$, then, $\hat{c}(x, 0) = f(k)$

This is demonstrated with the delta function. Given that a particle is fixed at the origin, the initial condition, or $f(k)$, is equal to 1 as the delta function and 1 is a Fourier pair.

$$c(x, t) = \int_{-\infty}^{\infty} \mathbf{exp} [-Dk^2 t] \mathbf{exp} [ikx] dk \quad (\text{A.9})$$

This is the inverse Fourier transform of the Gaussian function. Let $y = \sqrt{Dt}k$ and $\zeta = \frac{x}{\sqrt{Dt}}$

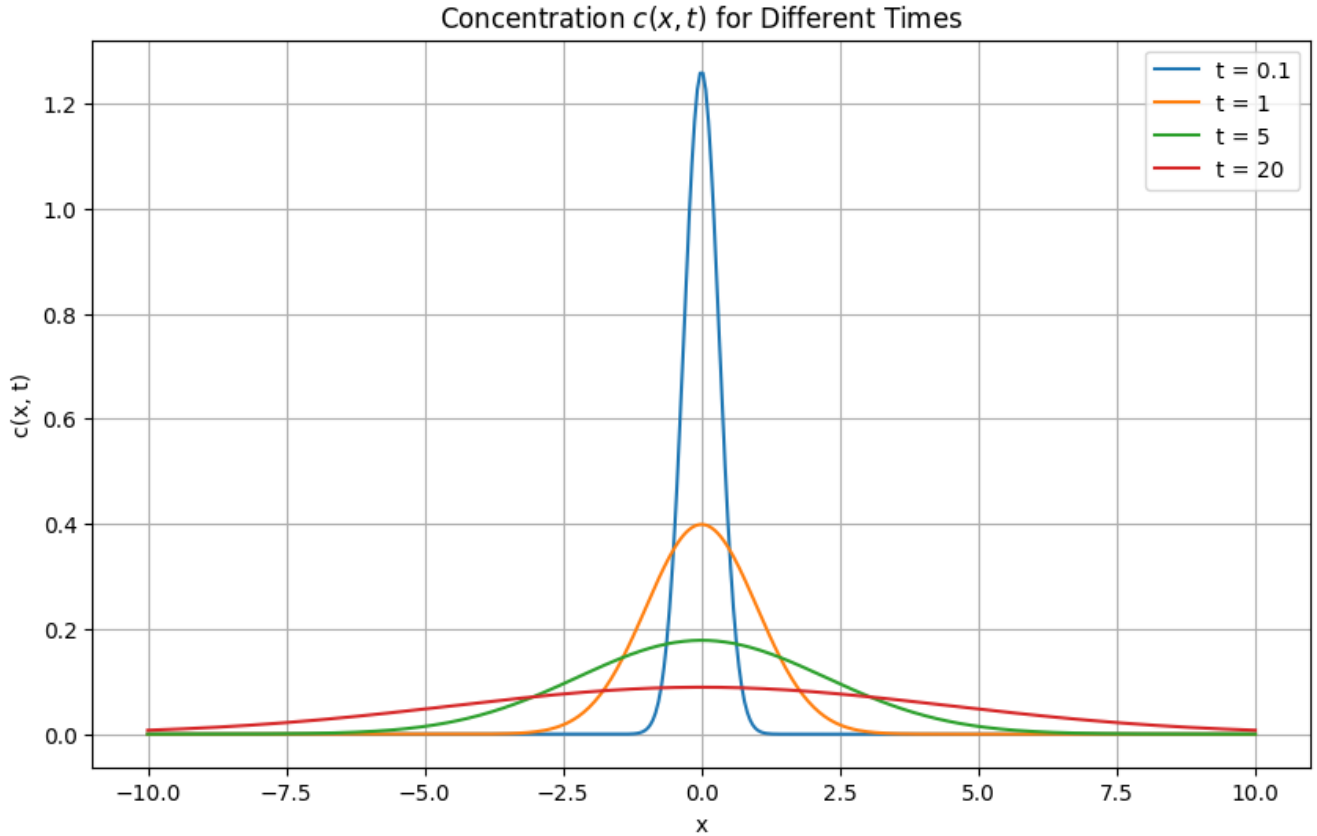
$$\begin{aligned} c(x, t) &= \frac{1}{2\pi\sqrt{Dt}} \int_{-\infty}^{\infty} \exp[-y^2] \exp[ik\zeta] dy \\ &\rightarrow \frac{1}{\sqrt{4\pi Dt}} \exp[-\zeta^2/4] \end{aligned} \quad (\text{A.10})$$

Thus, in its full glory:

$$c(x, t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left[-\frac{(x - x')^2}{4Dt}\right] \quad (\text{A.11})$$

Where x' denotes the initial position of the particle. This is generalized for any starting position, as the delta function is shift invariant in terms of the resultant Fourier transform other than a phase factor which is easily recognizable.

This can be simply plotted to visualize the distribution.



A.2. 1D CONFINED DIFFUSION EQUATION VIA SEPARATION OF VARIABLES

The boundaries of the problem are stated that at $0, L$, the boundaries are reflective: $\partial_x C(0, t) = \partial_x C(L, t) = 0$. Then, the diffusion equation can be read as:

$$\partial_t c(x, t) = D \partial_{xx} c(x, t) \quad (\text{A.12})$$

Using the method of separation of variables, the solution is proposed as $c(x, t) = X(x)T(t)$, which then gives the form as:

$$\frac{T'}{T} = D \frac{X''}{X} \quad (\text{A.13})$$

Since these equations are not of the same variables, but equal to themselves, they must be constants. The constant will have three forms, however, the time dependent form will be the same for each.

$$T(t) = \mathbf{exp}[-\lambda t] \quad (\text{A.14})$$

The x equation can be solved in terms of exponential. Let the solution be guessed as $\mathbf{exp}[rx]$. Denote $\gamma = \sqrt{\frac{\lambda}{D}}$

$$r^2 + \frac{\lambda}{D} = 0 \quad (\text{A.15})$$

If $\lambda = 0$, the solution is trivial and the solution is given as:

$$X_T(x) = Ax + B \quad (\text{A.16})$$

If $\lambda > 0$, the solution is given in terms of hyperbolic sines.

$$X_H(x) = A\sinh(\gamma x) + B\cosh(\gamma x) \quad (\text{A.17})$$

If $\lambda > 0$, the solution is given in terms of trigonometric sines.

$$X_S(x) = A\sin(\gamma x) + B\cos(\gamma x) \quad (\text{A.18})$$

Applying the boundary conditions, the hyperbolic term cancels as there can only be a zero at 0. The trivial solution takes the form: $X = A$, which simply implies that $A = 0$. This provides the first solution being a constant.

To manage the sines, can simply take derivatives.

$$\begin{aligned} X'_S &= -\gamma A \sin(\gamma x) + \gamma B \cos(\gamma x) \\ 0 &= B \cos(\gamma x), \quad B = 0 \\ 0 &= -\gamma A \sin(\gamma L), \quad \gamma = \frac{n\pi}{L} \end{aligned} \quad (\text{A.19})$$

So, the solution for x takes the simplified form of a cosine series:

$$X = \sum_{i=0}^N A_n \cos\left(\frac{n\pi}{L}x\right) \quad (\text{A.20})$$

The full solution is then given as:

$$C(x, t) = \sum_{i=0}^N A_n \mathbf{exp}\left[-D \left(\frac{n\pi}{L}\right)^2 t\right] \cos\left(\frac{n\pi}{L}x\right) \quad (\text{A.21})$$

Now, we can apply an initial condition to obtain a full solution. This will allow for a time-evolution of the diffusion concentration, or on a single-molecule level, the positional probability functions. This is due to the Fokker-Plank equations holding the same form for the diffusion equation.

Let the particle be found in the middle of the well:

$$C(x, 0) = \delta\left(x - \frac{L}{2}\right) \quad (\text{A.22})$$

The Fourier coefficient A_n can be found by applying an orthogonal integral.

$$\begin{aligned} C(x, 0) &= \delta\left(x - \frac{L}{2}\right) = \sum_{i=0}^N A_n \cos\left(\frac{n\pi}{L}x\right) \\ \int_0^L \delta\left(x - \frac{L}{2}\right) \cos\left(\frac{m\pi}{L}x\right) dx &= \int_0^L \sum_{i=0}^N A_n \cos\left(\frac{n\pi}{L}x\right) \cos\left(\frac{m\pi}{L}x\right) dx \end{aligned} \quad (\text{A.23})$$

The LHS of this equation is trivial. The RHS of this equation can be calculated using the fact that the product of cosines will be equal to 0 if $m \neq n$. If $m = n$, the integral can be evaluated by the following identity.

$$\int_{-\pi}^{\pi} \cos\left(\frac{m\pi}{L}x\right) \cos\left(\frac{n\pi}{L}x\right) dx = \pi \delta_{mn} \quad (\text{A.24})$$

Thus, the Fourier coefficient is evaluated.

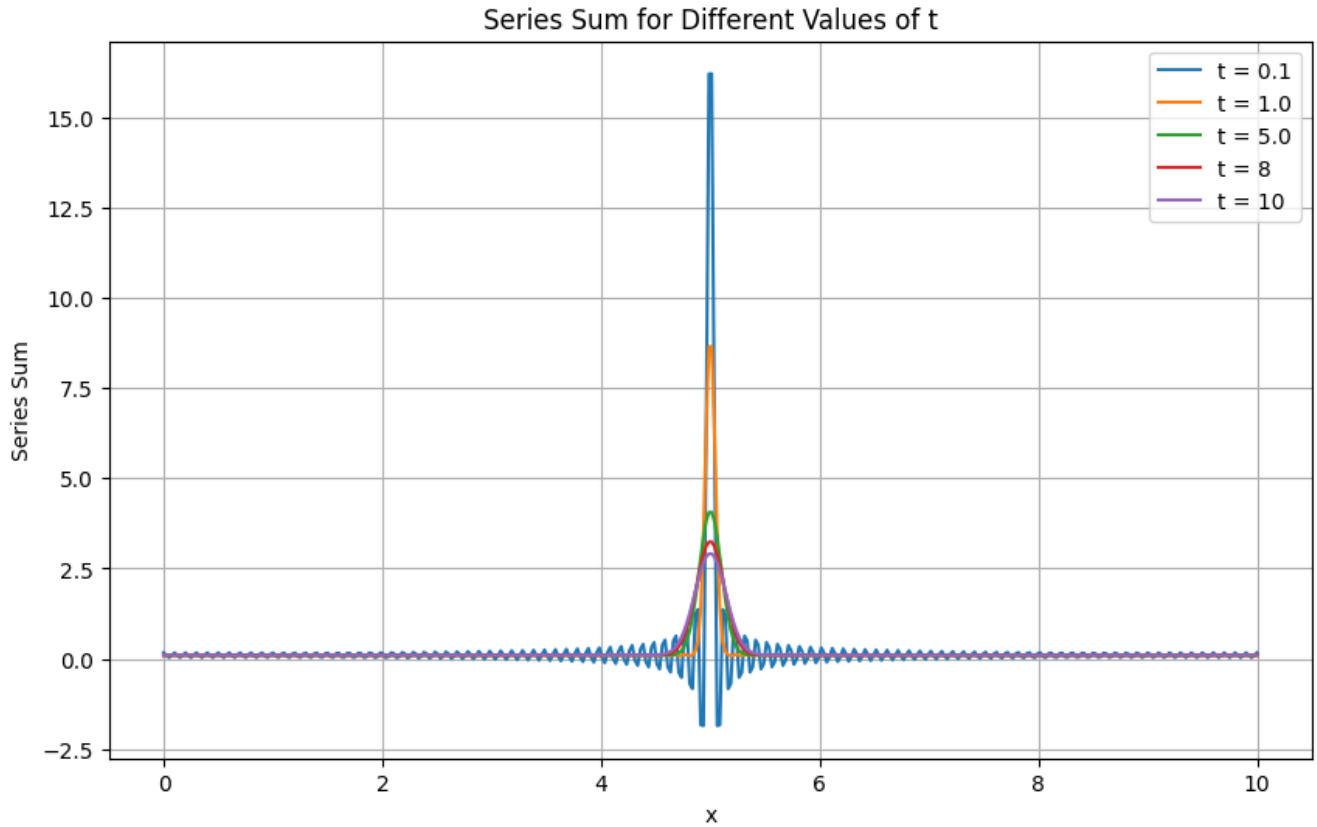
$$A_n \frac{L}{\pi} \int_0^{\pi} \cos(ny) \cos(my) dy = A_n \frac{L}{2} \quad (\text{A.25})$$

$$A_n = \frac{2}{L} \cos\left(\frac{n\pi}{L}x'\right)$$

Where x' is a generalized initial location of the particle. The series solution is then written as:

$$C(x, t) = \frac{2}{L} \sum_{n=0}^N \exp\left[-D \left(\frac{n\pi}{L}\right)^2 t\right] \cos\left(\frac{n\pi}{L}x\right) \cos\left(\frac{n\pi}{L}x'\right) \quad (\text{A.26})$$

To visualize this, the series solution is expanded upon and plotted at various timepoints:



A.3. 2D CONFINED DIFFUSION IN POLAR COORDINATES

The diffusion equation in polar coordinates is especially important due to applications in measuring **confined diffusion**. Solve the Diffusion equation with the following boundary equations:

$$\begin{aligned} \frac{\partial p(r, \phi, t)}{\partial r} \Big|_{r=a} &= 0 \\ p(r, 0, t) &= p(a, 2\pi, t) \end{aligned} \quad (\text{A.27})$$

First, the wave equation in polar coordinates is stated. Due to the polar geometry, the Laplacian undergoes the following transformations [2].

$$\nabla^2 = \partial_{rr} + \frac{1}{r}\partial_r + \frac{1}{r^2}\partial_{\phi\phi} \quad (\text{A.28})$$

The diffusion equation can then be stated:

$$\partial_t p(r, \phi, t) = D \left[\partial_{rr} p(r, \phi, t) + \frac{1}{r}\partial_r p(r, \phi, t) + \frac{1}{r^2}\partial_{\phi\phi} p(r, \phi, t) \right] \quad (\text{A.29})$$

To solve this, the method of separation of variables can be attempted. First, start by defining that:

$$p(r, \phi, t) = R(r)\Phi(\phi)T(t) \quad (\text{A.30})$$

Then, simply apply the Laplacian:

$$R\Phi T' = D \left[R''\Phi T + \frac{1}{r}R'\Phi T + \frac{1}{r^2}R\Phi''T \right] \quad (\text{A.31})$$

We can factor this equation into $\psi(r, \phi)$ and the time dependent $T(t)$:

$$\frac{T'}{T} = D \left[\frac{R''}{R} + \frac{1}{r}\frac{R'}{R} + \frac{1}{r^2}\frac{\Phi''}{\Phi} \right] \quad (\text{A.32})$$

Since each side doesn't depend on each other, they must be both equal to a constant; $-\lambda$.

$$\begin{aligned} \frac{T'}{T} &= -\lambda \\ D \left[\frac{R''}{R} + \frac{1}{r}\frac{R'}{R} + \frac{1}{r^2}\frac{\Phi''}{\Phi} \right] &= -\lambda \end{aligned} \quad (\text{A.33})$$

Before solving the equations, we can split this equation up one more time into Angular and Radial parts. By simply multiplying the second equation by r^2 , the equation can be separated into a second constant:

$$\begin{aligned} D \left[r^2 \frac{R''}{R} + r \frac{R'}{R} + \frac{\Phi''}{\Phi} \right] &= -\lambda r^2 \\ r^2 \frac{R''}{R} + r \frac{R'}{R} + \frac{1}{D} \lambda r^2 &= \frac{\Phi''}{\Phi} \end{aligned} \quad (\text{A.34})$$

So, the three equations to solve are:

$$\begin{aligned} \frac{\partial T}{\partial t} &= -\lambda T \\ r^2 \frac{\partial^2 R}{\partial r^2} + r \frac{\partial R}{\partial r} + R \left(\frac{1}{D} \lambda r^2 - \gamma^2 \right) &= 0 \\ \frac{\partial^2 \Phi}{\partial \phi^2} &= \gamma^2 \Phi \end{aligned} \quad (\text{A.35})$$

A.3.1. TIME-DEPENDENT EQUATION

The time dependent equation is the simplest to solve. This can be solved by solving the ODE. The general solution is listed below:

$$T(t) = T_0 \exp[-\lambda t] \quad (\text{A.36})$$

This is consistent with all other workings of the diffusion equation.

A.3.2. ANGULAR EQUATION

This equation is a simple linear 2nd order ODE. This can be solved by using the solution $\Phi = \exp[r\phi]$.

$$r^2 \exp[r\phi] - \gamma^2 \exp[r\phi] = 0 \quad (\text{A.37})$$

Thus, there will only be solutions depending on the sign of γ^2 . There are three cases. Each case must abide by the continuous and differentiable continuous BC of the angular components. Specifically, the equations must be 2π periodic. For $\gamma^2 = 0$, the solution is the linear:

$$\Phi = A\phi + b \quad (\text{A.38})$$

This cannot be periodic, so $A, B = 0$. For $\gamma^2 > 0$, the system will be a sum of exponents with real coefficients. This is equal to a sum of hyperbolics:

$$\Phi = A \sinh(\gamma\phi) + B \cosh(\gamma\phi) \quad (\text{A.39})$$

Same as in the first case, this cannot be periodic, hence, $A, B = 0$. For $\gamma^2 < 0$, the solution is the sum of imaginary exponentials, or a sum of sinusoids:

$$\Phi = A \exp[-i\gamma\phi] + B \exp[i\gamma\phi] \quad (\text{A.40})$$

A.3.3. RADIAL EQUATION

Let $\frac{\lambda}{D} = \psi^2$. Then, let $x = \psi r$. The equation will then become:

$$\frac{1}{x} \frac{\partial}{\partial x} \left(x \frac{\partial}{\partial x} R \right) + R \left(1 - \frac{\gamma^2}{x^2} \right) = 0 \quad (\text{A.41})$$

Expanding the LHS, the equation can be rewritten as a linear ODE:

$$\frac{\partial^2}{\partial x^2} R + \frac{1}{x} \frac{\partial}{\partial x} R + R \left(1 - \frac{\gamma^2}{x^2} \right) = 0 \quad (\text{A.42})$$

Since $x = 0$ is a singular point, which can be seen due to the divergence terms, the ODE can be solved using Frobenius methods. Thus, proposing a solution for $R(x)$:

$$R(x) = \sum_{n=0}^{\infty} a_n x^{n+s} \quad (\text{A.43})$$

This leads to the recursion relation that:

$$a_n = -\frac{a_{n-2}}{(n+s)^2 - \gamma^2} \quad (\text{A.44})$$

The fixed constants are a_0 and a_1 . We find that $a_1 = 0$, which stems from the requirement that $s = \pm\gamma$. Thus, the recursion relation solidifies itself as:

$$a_n = -\frac{a_{n-2}}{n(n+2\gamma)} \quad (\text{A.45})$$

This recursive relation can be solved via iteration with $n \rightarrow 2n$. Then, the solution that is forced upon all $n > 0$:

$$a_n = \left(-\frac{1}{4}\right)^n \frac{1}{n!(n+\gamma)!} a_0 \quad (\text{A.46})$$

By a careful choice of a_0 , this equation will form the general solution, which is known as the Bessel function of order γ .

$$J_\gamma(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(k+\gamma)!} \left(\frac{x}{2}\right)^{2k+\gamma} \quad (\text{A.47})$$

Thus, plugging in the value of x :

$$J_\gamma(r) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(k+\gamma)!} \left(\frac{\psi r}{2}\right)^{2k+\gamma} \quad (\text{A.48})$$

A.3.4. BOUNDARY CONDITIONS

The boundary conditions can now be applied. The boundary conditions for this problem are that there are vanishing derivatives at the edge of the boundary, as well as an angular symmetry:

$$\frac{\partial}{\partial r} p(r, \phi, t)|_{r=a} = 0 \quad (\text{A.49})$$

$$p(r, 0, t) = p(r, 2\pi, t) \quad (\text{A.50})$$

To apply the vanishing derivatives, we note that only the bessel functions will be dependent on r . Thus, the equation for the bessel function derivatives will vanish at 0.

$$J'_\gamma(a) = 0 \quad (\text{A.51})$$

This imposes that $x = \psi a$ must be the roots of the derivative of the Bessel function, which I will denote $z_{\gamma m}$.

$$\psi_{\gamma m} = \frac{z_{\gamma m}}{a} \quad (\text{A.52})$$

This imposes a condition on the previous constant λ . Recalling how λ is related to ψ we find that:

$$\lambda_{\gamma m} = D\psi^2 = D \frac{z_{\gamma m}^2}{a^2} \quad (\text{A.53})$$

Applying the condition that $p(r, 0, t) = p(r, 2\pi, t)$, we find that the angular portion may only contain values of γ in the integers.

$$Phi(\phi) = A\cos(\gamma\phi) + B\sin(\gamma\phi) \quad (\text{A.54})$$

This gives the general form of the solution:

$$p(r, \phi, t) \quad (\text{A.55})$$

The MSD of this solution is referenced in the following form [1]. This equation is important in the experimental context as it is often the form used in 2D microscope data.

$$\langle r^2 \rangle = a^2 \left(1 - 8 \sum_{m=1}^{\infty} \exp \left[-\alpha_{1m}^2 \frac{Dt}{a^2} \right] \frac{1}{\alpha_{1m}^2 (\alpha_{1m}^2 - 1)} \right) \quad (\text{A.56})$$

Where α_{1m} are the roots of the derivative of the 1st order Bessel function, a is the well radius, D is the diffusion, and t is a time step, or the exposure time.

When fitting experimentally, fitting a , D and an offset is required.

HOW TO DO FORMATTING WITH THIS PACKAGE

B.1. FORMATS

Nunc ante **bold** lectus, pretium id *italic* sodales, dapibus ~~strike through~~ urna. Suspendisse maximus underlined metus sed ante commodo efficitur. Some inline code: `def func(a,b): return a+b`

B.2. MATHEMATICS

Pellentesque sagittis orci ut lorem blandit, vel cursus urna interdum. Mauris malesuada fermentum ipsum, accumsan varius velit porttitor ut. Lorem ipsum dolor sit amet, consectetur adipiscing elit. Etiam rutrum sem orci, eget ornare justo sodales.

$$\hat{x}_i = \frac{x_i - \mu}{\sqrt{\sigma^2 + \varepsilon}} \tag{B.1}$$

B.3. CODE BLOCKS

Nullam congue ligula vitae urna convallis commodo. Proin nunc mi, vulputate quis viverra eu, consequat vitae risus sed venenatis. Praesent ut libero in dui mattis maximus.

```
.....
1 # Mauris viverra massa id lorem pretium gravida.
2
3 if num == 1:
4     print(num, "is not a prime.")
5 elif num > 1:
6     for i in range(2, num):
7         if (num % i) == 0:
8             print(num, "is a prime.")
9             break
.....
```

Snippet B.1: This is some code.

Cras vitae sem egestas, elementum felis vitae, ultricies ante. Fusce pellen tesque massa vitae massa molestie, at cursus urna scelerisque. Aliquam malesuada nunc at est vulputate condimentum. Cras fermentum nisi sit amet nulla pulvinar, vel vulputate ante tempor. Quisque vehicula nibh tortor, nec consectetur lorem semper sit amet.

B.4. TABLES

Interdum et malesuada fames ac ante ipsum primis in faucibus. Pellentesque eget mauris vitae metus pulvinar hendrerit nec non metus. Sed bibendum sapien non elit tempus accumsan. Phasellus in leo eu dui auctor laoreet. Etiam dui tellus, congue consequat accumsan nec, condimentum at est.

This	is	a	cool	table
1	2	3	4	5
a	b	c	d	e

Table B.1: This is a table - Notice that the description wraps.

B.5. FIGURES

Nullam massa nunc, sollicitudin id eleifend vitae, pellentesque sit amet lectus. Morbi vestibulum leo quis tempor lacinia. Praesent vitae est ante. Fusce dignissim in urna et posuere.

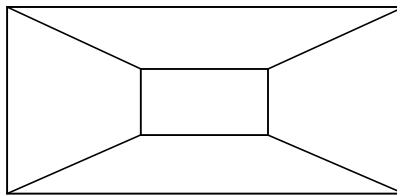


Figure B.1: This is an svg-figure scaled by 0.3, and this is a very long description.

Integer sed metus malesuada, volutpat urna condimentum, aliquet metus. Phasellus interdum.

B.6. LISTS

Elit vel sagittis luctus, arcu libero pellentesque nisi, sed consectetur quam neque a elit. Donec consectetur cursus nulla eu feugiat. Lorem ipsum dolor sit amet, consectetur adipiscing elit.

1. Something.
2. Another thing.
 - 2.1. A subitem.
 - 2.2. Another subitem.
 - A subitem.
 - Another subitem.
3. And another item.
4. Last item.

B.7. REFERENCING

Here is a [hyperlink to a webpage](#). This is a reference to equation B.1, and this refers to figure B.1. You can also refer to headings like section B.4. Snippet B.1 is a capitalized variant. For all references, both the name and number are links.

CONCLUSION

BIBLIOGRAPHY

- [1] BICKEL, T. A note on confined diffusion. *arXiv* (2007).
- [2] CRISTOFARO, R. The laplacian in polar and spherical coordinates.

