Section 3.4

Further Considerations Pertinent to the Relationship Between Probability and Partial Differential Equations

3.4.0 Introduction

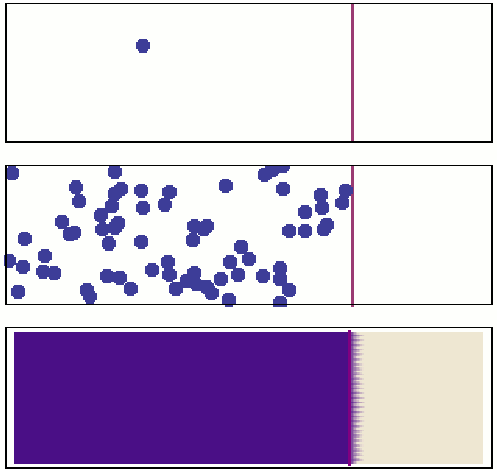
The partial differential equation of Brownian motion is common to various different phenomena

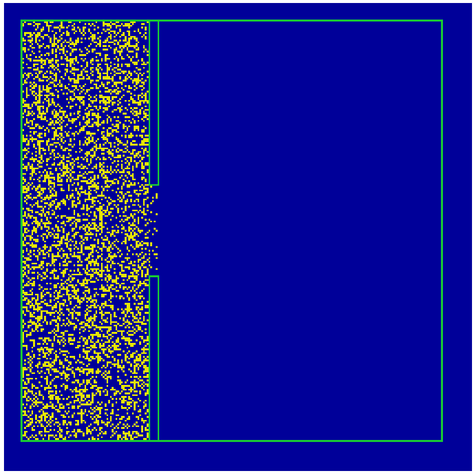
- heat conduction
- diffusion of gas

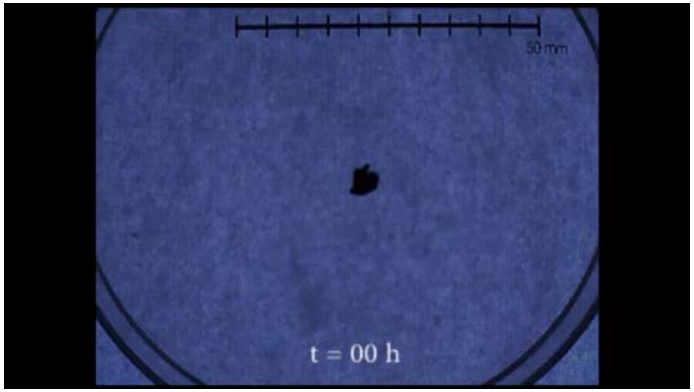
In this section, we will

- continue to study the relations between random walk and partial differential equations from a continuum viewpoint.
- examine various solution techniques for the diffusion equation.

3.4.1 More on diffusion equation and random walk







$$\boxed{J \propto -\nabla u}$$

- There is flow from high concentration to low concentration.
- The simplest hypothesis: such flow is due to difference in concentration.
- The magnitude of *flow* is proportional to *gradient.* This is Fick's first law.

To derivation from a continuum viewpoint

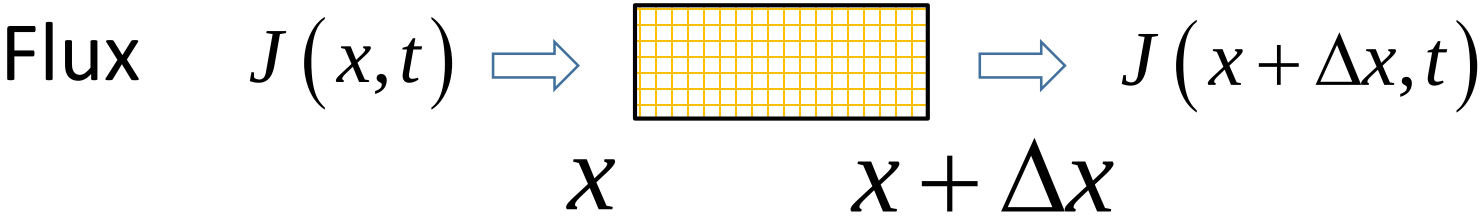
$$\boxed{\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}}$$

We start with

- $u(x, t)$ concentration: the amount per unit volume of some quantity interested.
- $J(x, t)$ flux: measuring the amount of substance that flow through a unit area during a unit time. Its dimension

[flux]=[quantity] / ([time]·[area])

3.4.1 More on diffusion equation and random walk



Flux $J(x,t) \Rightarrow$ $\Rightarrow J(x+\Delta x,t)$

x $x+\Delta x$

mass conservation:

$$\frac{\partial}{\partial t}\int_{x}^{x+\Delta x} u(x,t)dx = J(x,t) - J(x+\Delta x,t)$$

$$\Downarrow$$

$$\frac{\partial}{\partial t}\left[u(x,t)\Delta x\right] = J(x,t) - J(x+\Delta x,t)$$

$$\frac{\partial}{\partial t}u(x,t) = -\frac{J(x+\Delta x,t) - J(x,t)}{\Delta x}$$

$$\Downarrow$$

$\Delta x \to 0$

$$\boxed{\frac{\partial u}{\partial t} = -\frac{\partial J}{\partial x}}$$

3.4.1 More on diffusion equation and random walk

constitutive relation: Fick's first law

$$J = -D\frac{\partial u}{\partial x}$$

D diffusion constant.

$$\frac{\partial u}{\partial t} = -\frac{\partial J}{\partial x}$$

$$J = -D\frac{\partial u}{\partial x}$$

$$\Rightarrow \quad \boxed{\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}}$$

diffusion equation

u can be

- Temperature
- Concentration
- …

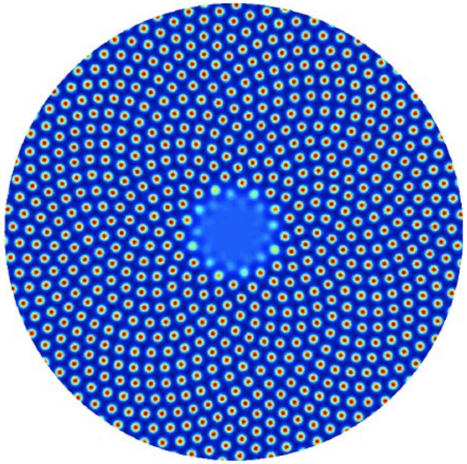
Comments

- macro diffusion time $t \gg$ particle collision time τ
- macro diffusion distance $\gg$ particle mean free path
- macro diffusion velocity $\ll$ particle velocity

Nonlinear Diffusion Models

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + f\left(u\right)$$

Phyllotaxis



$$\frac{\partial u}{\partial t} = \mu u - (\nabla^2 + 1)^2 u - \frac{\beta}{3}(|\nabla u|^2 + 2u\nabla^2 u) - u^3,$$

Alan C. Newell. PRL 110, 248104 (2013)

3.4.1 More on diffusion equation and random walk

We seek the solution of

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + f\left(u\right) \xrightarrow{x \to x/\sqrt{D}} \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + f\left(u\right)$$

normal (Fourier) modes

$$u\left(k\right) = A\left(k\right)e^{i\left(kx-\omega t\right)}$$

the solution

$$u\left(x,t\right) = \int_{-\infty}^{\infty} A\left(k\right)\exp\left[ikx - i\omega t\right]dk$$

3.4.1 More on diffusion equation and random walk

- When $f(u) = 0$ $\quad u_t = u_{xx}$

$$u_t = -i\omega u \qquad u_{xx} = -k^2 u \quad \Rightarrow$$

Dispersion relation $\quad \omega = -ik^2$

Phase velocity $\quad c = \mathrm{Re}(\omega)/k = 0$

$$u(k) = A(k)\exp\left(ikx - k^2 t\right) = A\underline{\exp\left(-k^2 t\right)}\exp(ikx)$$

$\Downarrow$

decay quickly as k>>1

$$u \to 0 \quad as\; t >> 1$$

Called: dissipation

No constant wave in diffusion equation

3.4.1 More on diffusion equation and random walk

- When $f(u) = au_x + bu$ $\quad u_t = u_{xx} + au_x + bu$

$$a, b > 0$$

Dispersion relation $\omega = -ak - i\left(k^2 - b\right)$

Phase velocity $c = \mathrm{Re}\left(\omega\right)/k = -a$

$$u(k) = Ae^{-\left(k^2 - b\right)t}\exp\left[ik\left(x + at\right)\right]$$

$t >> 1$ decay quickly as $\boxed{k \neq \pm b}$

$k = \pm b$

⬇

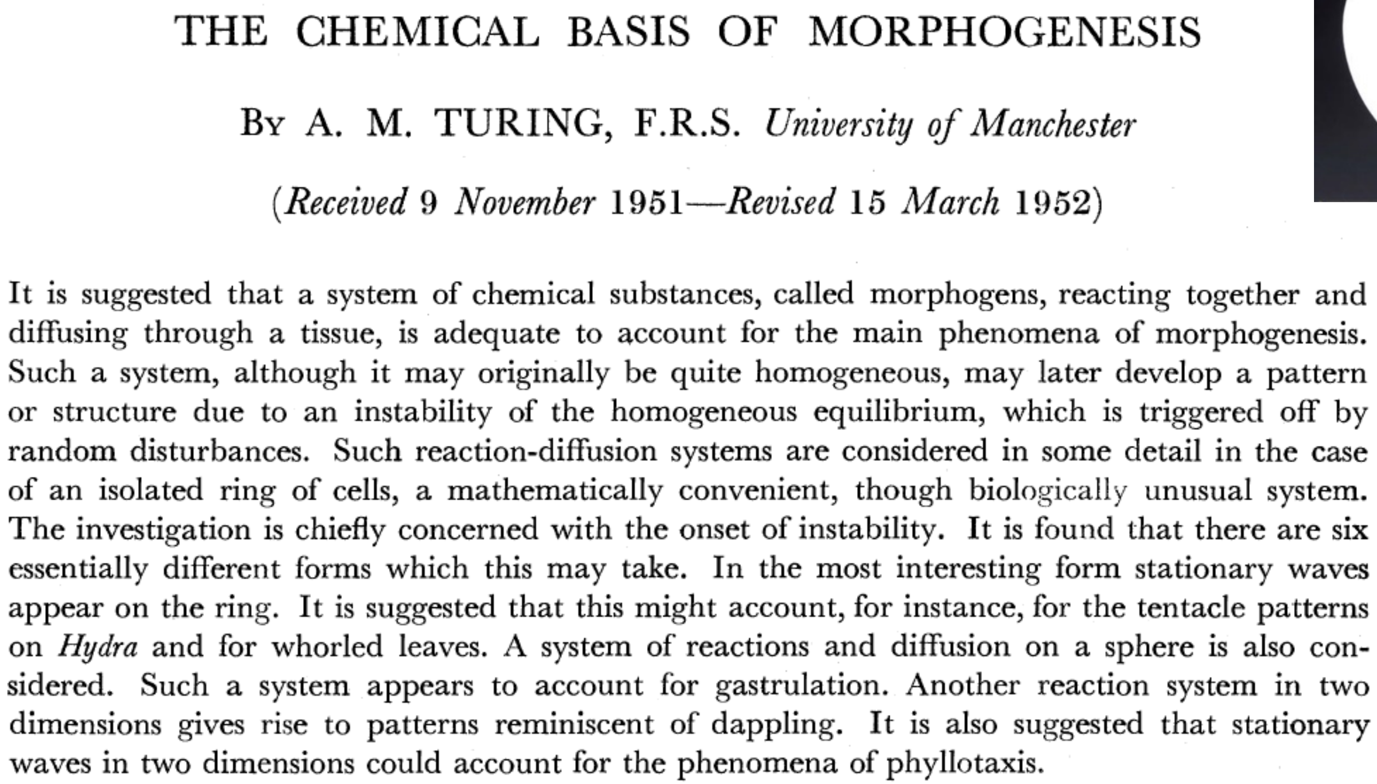
$$u = A\exp\left[\pm ib\left(x + at\right)\right]$$

Two constant waves

Nonlinear reaction diffusion models

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + f\left(u,v\right) \qquad \frac{\partial v}{\partial t} = D\frac{\partial^2 v}{\partial x^2} + g\left(u,v\right)$$

Turing Patterns

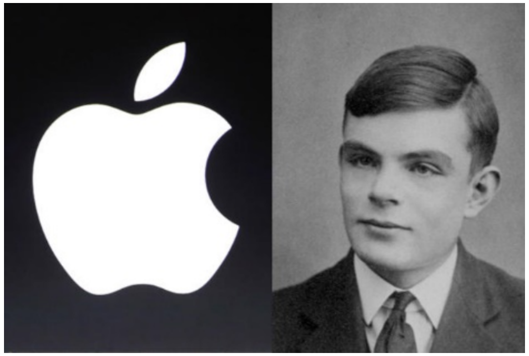


THE CHEMICAL BASIS OF MORPHOGENESIS

By A. M. TURING, F.R.S. *University of Manchester*

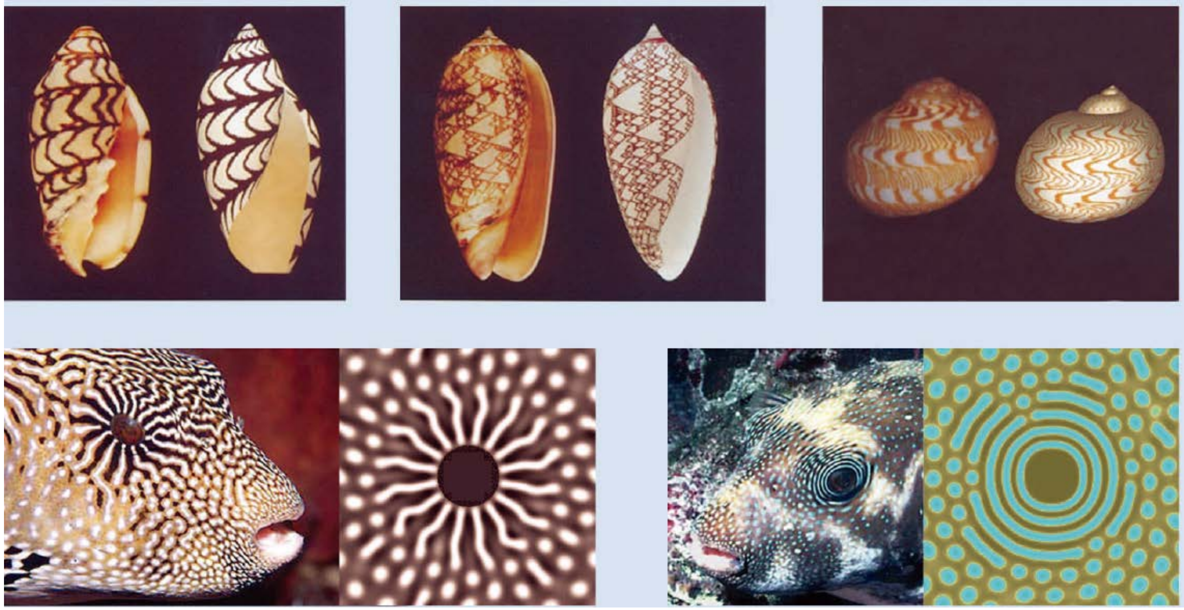
(*Received* 9 *November* 1951—*Revised* 15 *March* 1952)

It is suggested that a system of chemical substances, called morphogens, reacting together and diffusing through a tissue, is adequate to account for the main phenomena of morphogenesis. Such a system, although it may originally be quite homogeneous, may later develop a pattern or structure due to an instability of the homogeneous equilibrium, which is triggered off by random disturbances. Such reaction-diffusion systems are considered in some detail in the case of an isolated ring of cells, a mathematically convenient, though biologically unusual system. The investigation is chiefly concerned with the onset of instability. It is found that there are six essentially different forms which this may take. In the most interesting form stationary waves appear on the ring. It is suggested that this might account, for instance, for the tentacle patterns on *Hydra* and for whorled leaves. A system of reactions and diffusion on a sphere is also considered. Such a system appears to account for gastrulation. Another reaction system in two dimensions gives rise to patterns reminiscent of dappling. It is also suggested that stationary waves in two dimensions could account for the phenomena of phyllotaxis.



23 June 1912
– 7 June 1954

Turing Patterns



3.4.2 Superposition of fundamental solutions: the method of images

Diffusion equation $$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}$$

solution $$u_0(x,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right)$$

satisfy

- delta function initial condition

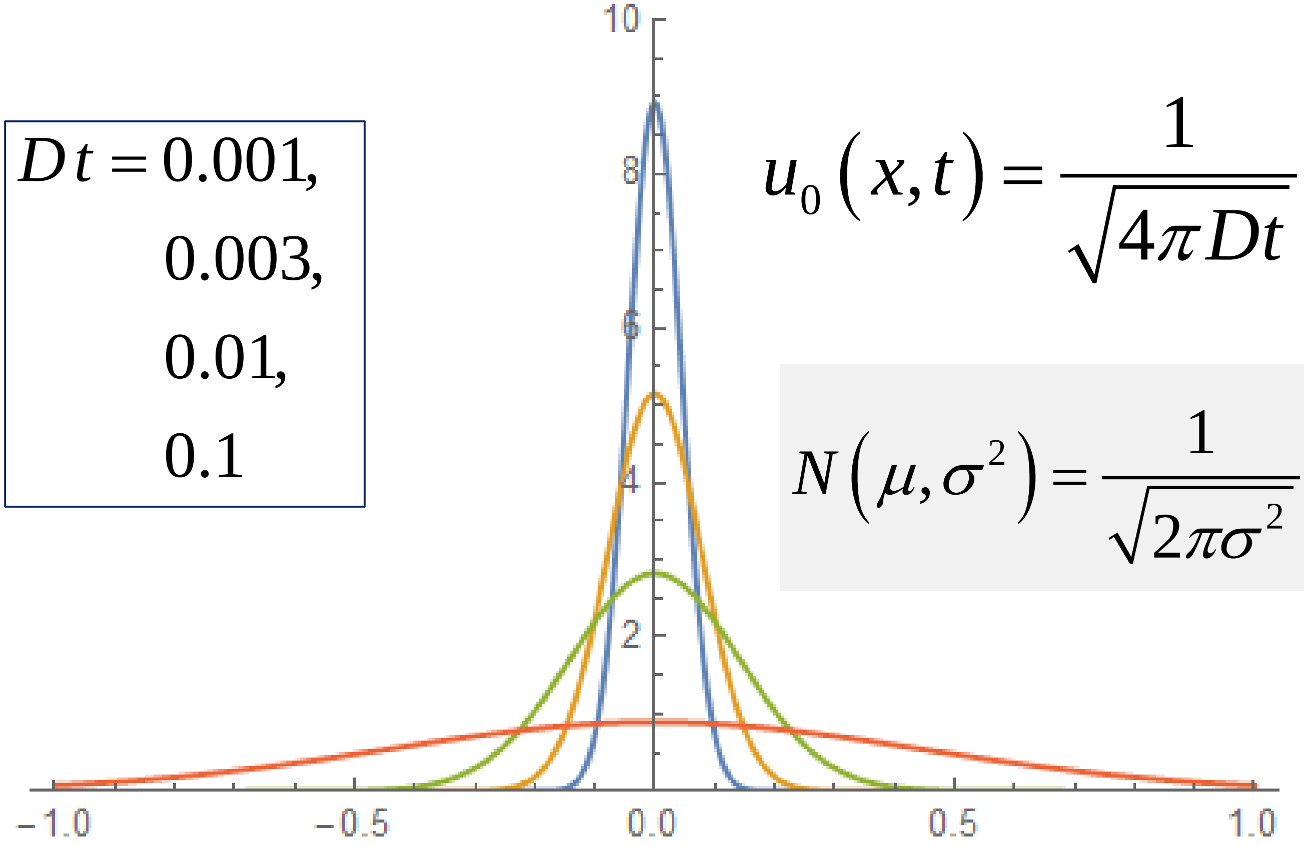
$$\lim_{t\to 0^+} u_0(x,t) = 0, \qquad x \neq 0$$

$$\int_{-\infty}^{\infty} \delta(x)\,dx = 1$$

- normalization condition

$$\int_{-\infty}^{\infty} u_0(x,t)\,dx = 1$$

3.4.2 Superposition of fundamental solutions: the method of images



$$u_0(x,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$$

$$N(\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

- $u_0(x,t)$ called unit source solution or fundamental solution.
- general solution formed from its combinations.

Some properties of the diffusion equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}$$

- Translation invariance

$u_0\left(x,t\right)$ is a solution

$$x \to x-\xi, \qquad t \to t-\tau$$

$u_0\left(x-\xi, t-\tau\right)$ also solution

an unit source initially placed at point ξ and time τ.

3.4.2 Superposition of fundamental solutions: the method of images

- Linearity and superposition

$$u(x,t) = c_1 u_1(x,t) + c_2 u_2(x,t)$$

The combination of solutions is also a solution.

$u_0(x,t)$ is a solution of $\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}$

$$u(x,t) = c_1 u_0(x-\xi_1,t) + c_2 u_0(x-\xi_2,t)$$

superposition of two sources

Reflecting barrier

$$\begin{cases} \dfrac{\partial u}{\partial t} = D\dfrac{\partial^2 u}{\partial x^2} \\ \displaystyle\int_{-\infty}^{L} u(x,t)dx = 1 \\ \displaystyle\lim_{t\to 0^+} u(x,t) = 0, \qquad x \neq 0 \\ u_x(L,t) = 0 \end{cases}$$

$$\begin{aligned} u &= u_{\mathrm{R}}(x,t) \\ &= u_0(x,t) + u_0(x-2L,t) \end{aligned}$$

Absorbing barrier

$$\begin{cases} \dfrac{\partial u}{\partial t} = D\dfrac{\partial^2 u}{\partial x^2} \\ \cancel{\displaystyle\int_{-\infty}^{L} u(x,t)dx = 1,} \\ \displaystyle\lim_{t\to 0^+} u(x,t) = 0, \qquad x \neq 0 \\ u(L,t) = 0 \end{cases}$$

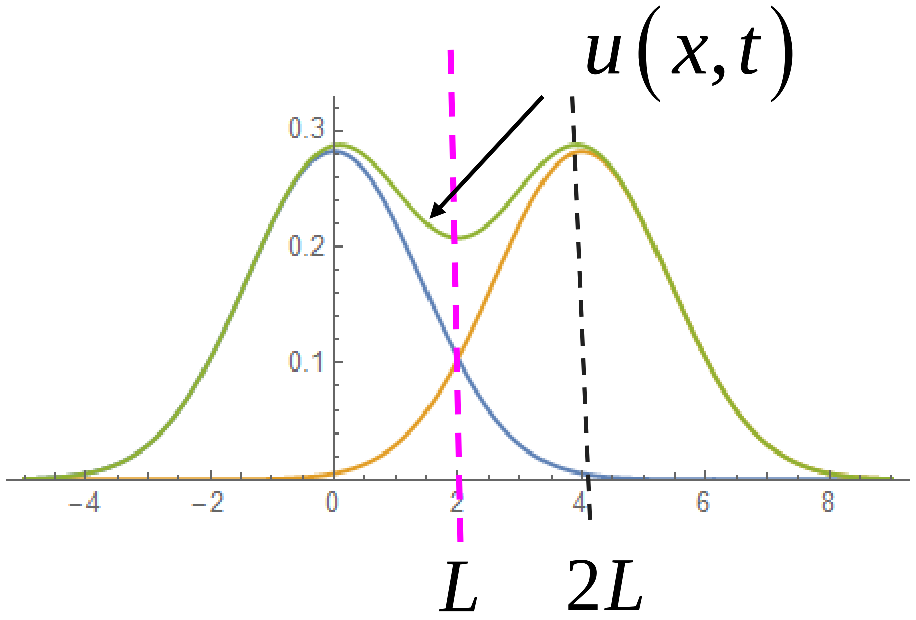
$$\begin{aligned} u &= u_{\mathrm{A}}(x,t) \\ &= u_0(x,t) - u_0(x-2L,t) \end{aligned}$$

u_0 fundamental solution starting at x=0 and t=0

Method of image 镜像法

Reflecting barrier

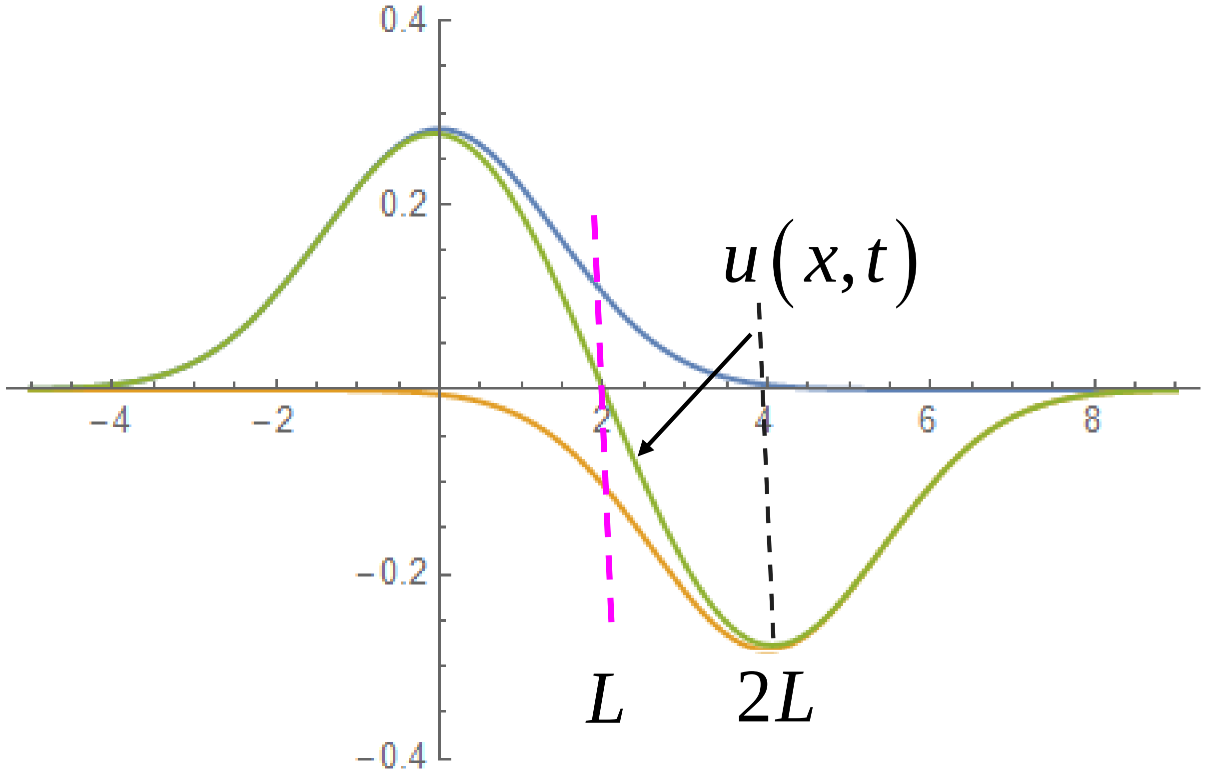
Boundary condition $u_x(L,t)=0$



$$u(x,t)=u_0(x,t)+u_0(x-2L,t)$$

Absorbing barrier

Boundary condition $u(L,t)=0$



$$u(x,t)=u_0(x,t)-u_0(x-2L,t)$$

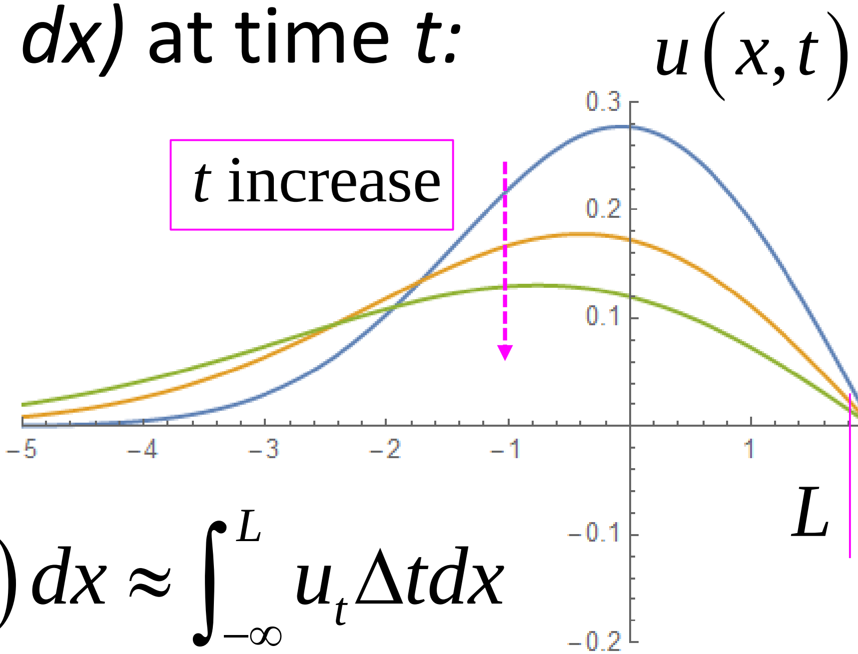
3.4.3 First passage time as a flux

Consider the leaking probability at the boundary x=L of absorbing barrier

$$u(x,t) = u_0(x,t) - u_0(x-2L,t) \qquad u(L,t) = 0$$

Probability between (*x*, *x* + *dx*) at time *t:*

$$\int_x^{x+\Delta x} u(x,t)\,dx$$



The total probability *U*(*t*)

$$\Delta U = \int_{-\infty}^{L} u(x,t+\Delta t) - u(x,t)\,dx \approx \int_{-\infty}^{L} u_t \Delta t\,dx$$

$$\frac{\partial U}{\partial t} = \int_{-\infty}^{L} \frac{\partial u}{\partial t}\,dx = \int_{-\infty}^{L} D\frac{\partial^2 u}{\partial x^2}\,dx = D\left(\frac{\partial u}{\partial x}\right)_L$$

3.4.3 First passage time as a flux

- Define *F(L, t) dt* the probability that a particle is absorbed (flow out) per unit time at *x* = *L* in the time interval *(t, t + dt)*

$$F(L,t)\,dt = -\frac{\partial U}{\partial t}dt = -D\left(\frac{\partial u}{\partial x}\right)_L dt$$

- An alternative interpretation of *F(L, t) :* the rate at which mass is leaving the system at *x* = *L.*

$$F(L,t) = -D\left(\frac{\partial u_A}{\partial x}\right)_L = J(L,t)$$

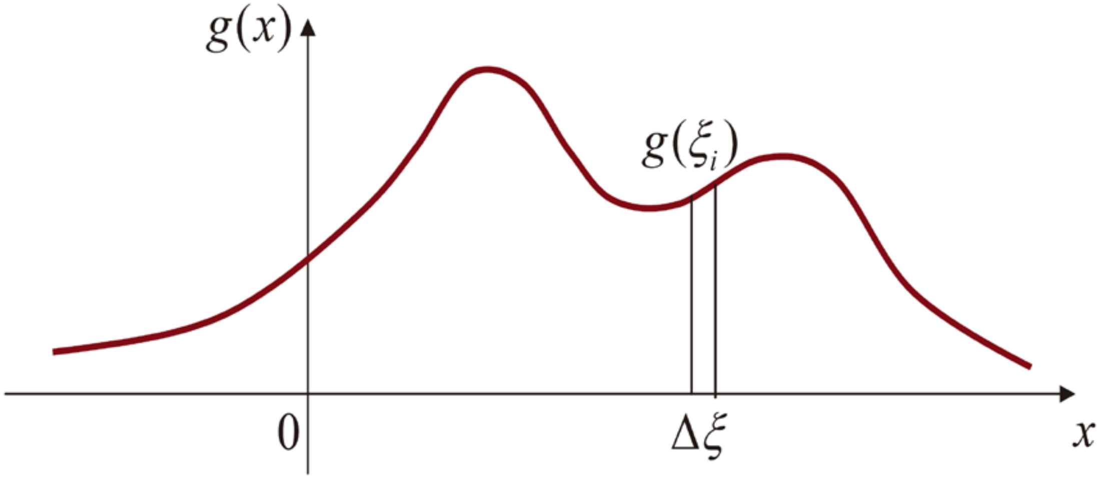
3.4.4 General initial value problem in diffusion

Consider $\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}$

with initial condition

$$u\left(x,0\right) = g\left(x\right)$$

with $-\infty < x < \infty$



The solution can be linear superposition of fundamental solution

$$u\left(x,t\right) = \int_{-\infty}^{\infty} u_0\left(x-\xi,t\right) g\left(\xi\right) d\xi$$

$$g\left(x\right) \to 0, \qquad \text{as} \;\; x \to \pm\infty$$

convolution

$$f\left(x\right) * g\left(x\right) = \int_{-\infty}^{\infty} g\left(x-\xi\right) f\left(\xi\right) d\xi$$

3.4.4 General initial value problem in diffusion

To check the initial condition $u(x,0)=g(x)$

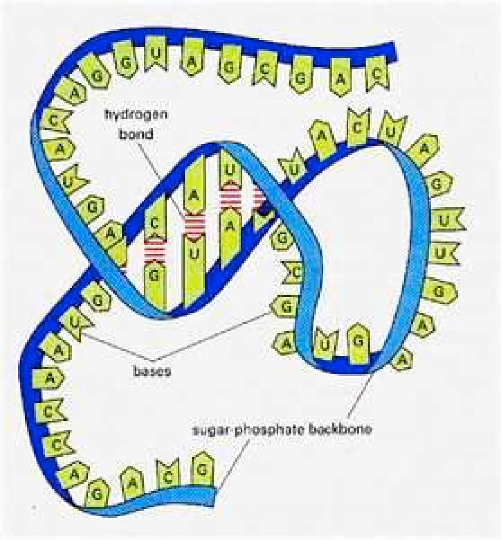
$$u(x,t)=\int_{-\infty}^{\infty} u_0(x-\xi,t)\,g(\xi)\,d\xi$$

$$=\int_{-\infty}^{\infty}\frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{(x-\xi)^2}{4Dt}\right)g(\xi)\,d\xi \qquad \eta^2=\frac{(x-\xi)^2}{4Dt}$$

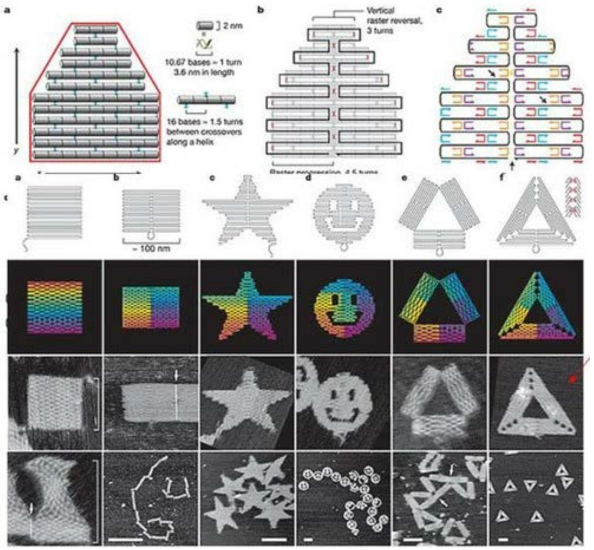
$$=\int_{-\infty}^{\infty}\frac{1}{\sqrt{\pi}}\exp\left(-\eta^2\right)g\left(x+\eta\sqrt{4Dt}\right)d\eta$$

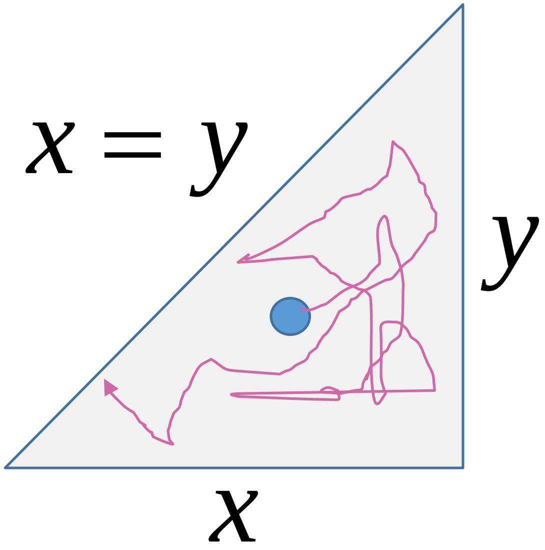
$$\lim_{t\to 0^+} u(x,t)=g(x)$$

3.4.5 DNA and The first passage in 2D

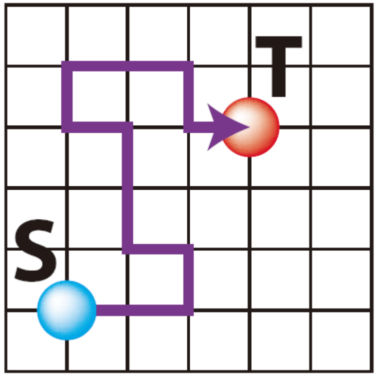


DNA origami - DNA as a structural

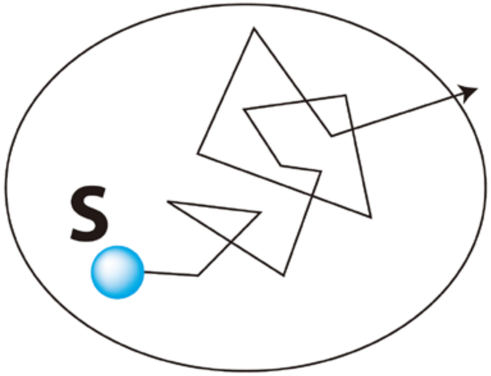




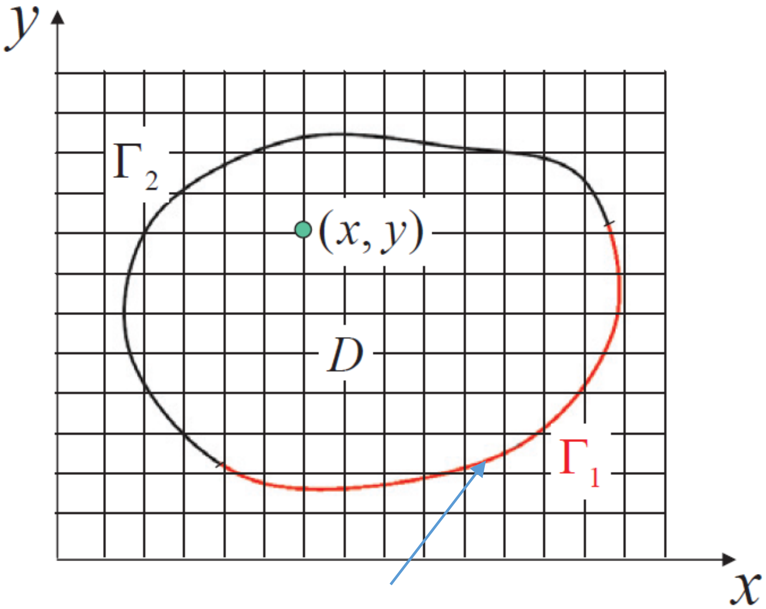
3.4.5 DNA and The first passage in 2D



first-passage



first-exit

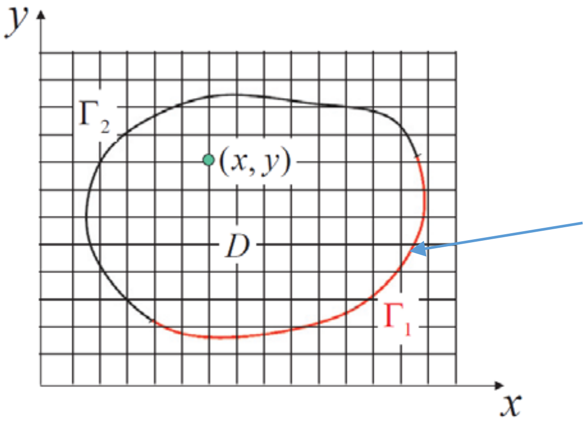


Absorbing boundary

To determine the probability *$P(x, y)$:*

- *a particle* starting from a point (x,y) in region D
- first reaching the absorbing boundary Γ_1.

3.4.5 DNA and The first passage in 2D



Discrete boundary point (x_i, y_i)

we obtain the partial difference equation

$$P(x, y)$$

$$=\frac{1}{4}\left[P(x-\Delta, y)+P(x+\Delta, y)+P(x, y-\Delta)+P(x, y+\Delta)\right]$$

If the starting point (x,y) is a boundary point, we have

$$P(x, y)=\begin{cases}1, & (x, y)=(x_i, y_i)\\ 0, & (x, y)\neq(x_i, y_i)\end{cases}$$

3.4.5 DNA and The first passage in 2D

Taylor expansion

⇩

Laplace equation

$$\frac{\partial^2 P}{\partial x^2}+\frac{\partial^2 P}{\partial y^2}=0$$

P: the probability density

Boundary conditions

$$\lim_{(x,y)\to\Gamma_1} P(x,y)=1$$

$$\lim_{(x,y)\to\Gamma_2} P(x,y)=0$$

$$\oint_{\Gamma} P(x,y)\,ds=\oint_{\Gamma_1}+\oint_{\Gamma_2} P(x,y)\,ds=\oint_{\Gamma_1} P(x,y)\,ds=1$$

3.4.5 DNA and The first passage in 2D

- Suppose f(x,y) the initial probability distribution function in *D*
- the probability that a particle leaving *D* along Γ_1 is

$$\bar{P} = \iint\limits_D P(x,y) f(x,y)\, dxdy$$

Noticing the *Green's second theorem*

$$\iint\limits_D \left(Q\nabla^2 P - P\nabla^2 Q\right) dxdy = \oint\limits_\Gamma \left(Q\frac{\partial P}{\partial n} - P\frac{\partial Q}{\partial n}\right) ds$$

$\frac{\partial}{\partial n}$ denotes exterior normal derivative

3.4.5 DNA and The first passage in 2D

- P is the probability function defined above
- Q is defined as

$$\nabla^2 Q = f, \qquad Q = 0 \ \text{ on } \ \Gamma$$

Using the *Green's second theorem*

$$\iint_D \left(Q\cancel{\nabla^2 P} - P\nabla^2 Q \right) dxdy = \iint_D \left(-P\,f \right) dxdy$$

$$= \oint_\Gamma \left(Q\cancel{\frac{\partial P}{\partial n}} - P\frac{\partial Q}{\partial n} \right) ds = \oint_\Gamma \left(-P\frac{\partial Q}{\partial n} \right) ds$$

$$\bar{P} = \iint_D P\,f\,dxdy = \oint_{\Gamma_1} P\frac{\partial Q}{\partial n} ds$$

3.4.5 DNA and The first passage in 2D

Now our questions becomes to solve *Q*

Poisson equation

$$\nabla^2 Q = f, \qquad Q = 0 \ \text{on} \ \Gamma$$

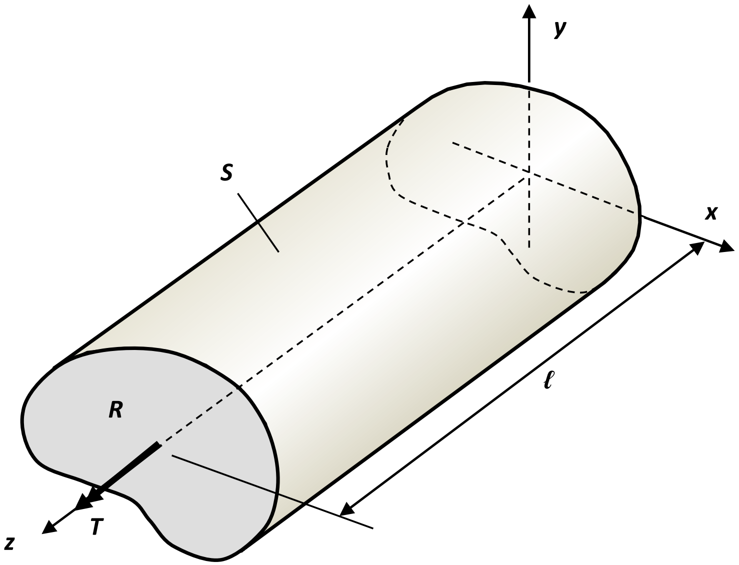
Then we can determine

$$\bar{P} = \int_{\Gamma_1} P\left(\frac{\partial Q}{\partial n}\right) ds$$

Example: Torsional Deformation

Stress Function $\phi = \phi(x,y)$

$$\tau_{xz} = \frac{\partial \phi}{\partial y}, \quad \tau_{yz} = -\frac{\partial \phi}{\partial x}$$



$$\nabla^2 \varphi = -2\mu\alpha$$

α *twist angle per length*

μ *Shear modulus*

3.4.6 Recurrence property in Brownian motion

A particle starts at a point *x* in the domain *D* described by

$$D:\varepsilon < x < R$$

1D Laplace equation

$$\frac{d^2P(x)}{dx^2} = 0$$

Boundary conditions

$$P = 1, \ \ as \quad |x| = \varepsilon$$

$$P = 0, \ \ as \quad |x| = R$$

Solution

$$P = \frac{R - |x|}{R - \varepsilon}$$

3.4.6 Recurrence property in Brownian motion

$$P = \frac{R - |x|}{R - \varepsilon} \to 1, \quad as\ R \to \infty, \quad x, \varepsilon\ \ fixed$$