LIÈGE université
Sciences Appliquées

Lecture 6 Diffusion equation

Mathématiques appliquées (MATH0504-1)

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Learning objectives

Find out that the diffusion equation has a number of invariance properties

Derive an explicit formula for the solution of the diffusion problem in an infinite domain

Become familiar with the concept of *source function*, or *Green's function*, or *fundamental solution* of the diffusion problem

Highlight the contrasting properties of the wave equation and the diffusion equation

Outline

1. Reminder

2. Solution of the diffusion equation, and IVP,
   in an infinite domain (incl. invariance properties)

3. Concept and properties of Green's function,
   or fundamental solution of the diffusion equation

4. Comparison between the solutions
   of the wave and the diffusion equations

Reminder

We study the 1D diffusion equation:

$$u_t = k u_{xx}$$

Maximum principle

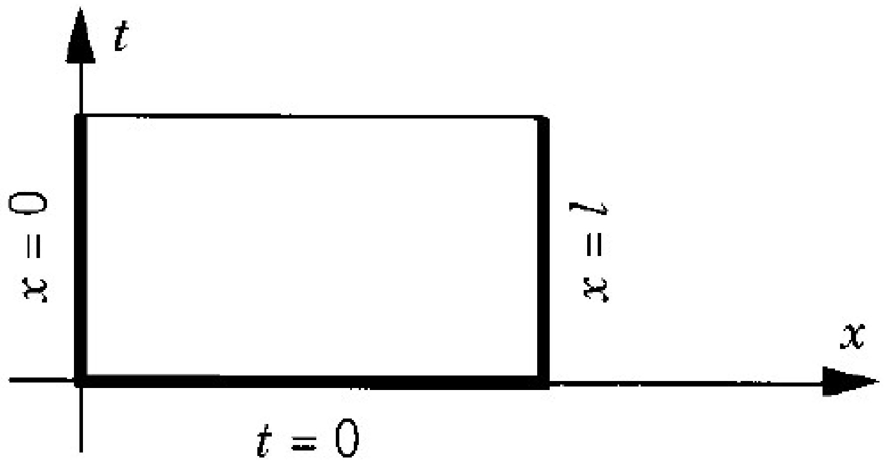
Stability

Uniqueness

Maximum principle

If $u(x, t)$ satisfies the diffusion equation in a rectangle (say, $0 \leq x \leq l$, $0 \leq t \leq T$) in space-time, then the maximum value of $u(x, t)$ is found

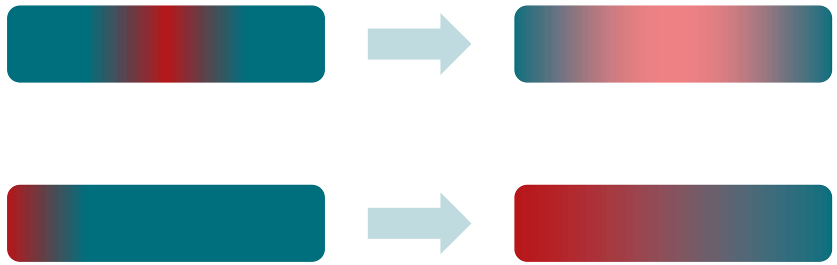
- either initially ($t = 0$)
- or on the lateral sides ($x = 0$ or $x = l$).



The maximum principle has a natural interpretation e.g. in terms of heat flow or diffusion of constituent

If you have a rod with no internal heat source, the hottest spot and the coldest spot can occur only initially or at one of the two ends of the rod.

- Thus a hot spot at time zero will cool off.
- You can burn one of its ends but the maximum temperature will always be at the hot end.



Similarly, if you have a substance diffusing along a tube, its highest concentration can occur only initially or at one of the ends of the tube.

The diffusion equation tends to smooth the solution out, which contrasts with the wave equation

Also the minimum value can be attained only on the bottom or the lateral sides.

To prove the “minimum” principle, just apply the maximum principle to $-u(x, t)$.

Consequence:

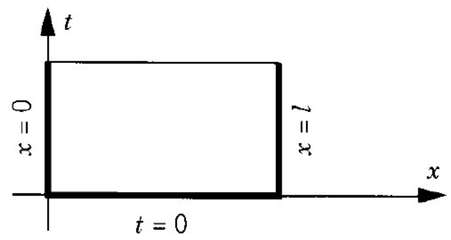
- the maximum drops down ↘
- while the minimum comes up. ↗

Uniqueness of the solution for the Dirichlet problem for the diffusion equation

There is at most one solution of

$$
\begin{aligned}
u_t - ku_{xx} &= f(x,t) \quad \text{for } 0 < x < l \text{ and } t > 0 \\
u(x,0) &= \phi(x) \\
u(0,t) &= g(t) \qquad u(l,t) = h(t)
\end{aligned}
$$

for four given functions f, ϕ, g, and h.



Uniqueness means that any solution is determined completely based on proper ICs and BCs.

Proof: from energy, or based on the maximum and minimum principles for $w = u_1 - u_2$, with $u_1(x, t)$, $u_2(x, t)$ two solutions.

Stability of the solution can be proven by the maximum principle, or from energy considerations

Consider two solutions $u_1(x, t)$ and $u_2(x, t)$ of the diffusion problem in a rectangle, for which

- $w \equiv u_1 - u_2 = 0$ on the lateral sides of the rectangle
- $w = \phi_1 - \phi_2$ on the bottom.

The maximum principle asserts that throughout the rectangle

$$u_1(x, t) - u_2(x, t) \leq \max|\phi_1 - \phi_2|$$

The "minimum" principle says that

$$u_1(x, t) - u_2(x, t) \geq -\max|\phi_1 - \phi_2|$$

Stability of the solution can be proven by the maximum principle, or from energy considerations

Therefore,

$$\max_{0 \le x \le l} |u_1(x,t) - u_2(x,t)| \le \max_{0 \le x \le l} |\phi_1(x) - \phi_2(x)|$$

valid for all $t > 0$. In this inequality,

- the right side is a quantity that measures the nearness of the initial data for two solutions,
- and on the left we measure the nearness of the solutions at any later time.

Thus, "if we start nearby (at $t = 0$), we stay nearby".

This is exactly the meaning of stability!

1 – Diffusion on the whole line

In this section, we derive the mathematical solution of the diffusion problem on an infinite domain (Section 2.4 in Strauss, 2008).

Diffusion problem on an infinite domain

Our purpose in this section is to solve the problem

$$u_t = ku_{xx} \quad (-\infty < x < \infty,\ 0 < t < \infty)$$
$$u(x, 0) = \phi(x).$$

Similarly as with the wave equation, the problem on the infinite line is

- easier to solve than the finite-interval problem
- and it is of practical relevance in some instances.

The effect of boundaries will be discussed later.

The derivation of the solution will be based on a method *very different* from those used so far

Our method is

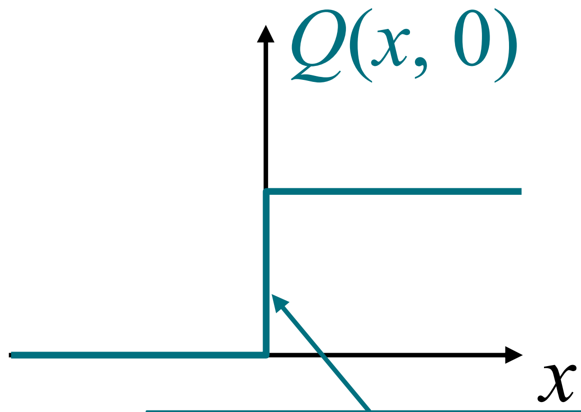
① • to solve it for a particular *initial condition* $\phi(x)$

② The particular solution we will look for is

③ denoted $Q(x, t)$, which satisfies the special IC:

$$Q(x,0) = 1 \quad \text{for } x > 0$$

$$Q(x,0) = 0 \quad \text{for } x < 0.$$



Implications of this discontinuity will be discussed later.

④ • and then build the general solution from this particular one.

We will use five basic invariance properties of the diffusion equation

❶ The translate $u(x-y, t)$ of any solution $u(x, t)$ is another solution for any fixed y.

- Consider $v(x, t) = u(x-y, t)$
- By the chain rule: $v_t = u_t$ and $v_{xx} = u_{xx}$; hence $v_t = k\, v_{xx}$

❷ Any derivative (u_x or u_t or u_{xx}, etc.) of a solution is again a solution.

- For instance, derive the diffusion equation with respect to x (or t): $u_{xt} = k\, u_{xxx}$ (or $u_{tt} = k\, u_{txx}$);
- Rename $v = u_x$ (or $v = u_t$)
- You end up with: $v_t = k\, v_{xx}$

Invariant ❷ uses the equality of mixed partials

If k is any positive integer, a function is said to be of class C^k if each of its partial derivatives of order $\leq k$ exists and is continuous.

If a function $f\,(x, y)$ is of class C^2, then

$$f_{xy} = f_{yx}.$$

The same is true for derivatives of any order. Although pathological examples can be exhibited for which the mixed derivatives are not equal, this lies out of the scope of this course.

We will use five basic invariance properties of the diffusion equation

❸ A linear combination of solutions is again a solution.

- This is just a consequence of linearity.

❹ An integral of solutions is again a solution.

- If $S(x, t)$ is a solution, then so is $S(x-y, t)$
- And so is

$$v(x,t) = \int_{-\infty}^{\infty} S(x-y,t)g(y)\,dy$$

for any function $g(y)$, as long as the integral converges.

- This is just a limiting form of ❸.

We will use five basic invariance properties of the diffusion equation

❺ If $u(x, t)$ is a solution, so is the dilated function

$$u(a^{1/2}\, x,\, a\, t), \text{ for any } a > 0.$$

- Prove this by the chain rule.
- Let $v(x, t) = u(a^{1/2}\, x, a\, t)$.
- Then $v_t = [\partial(a\, t)/\partial t]\, u_t = a\, u_t$
  and $v_x = [\partial(a^{1/2}\, x)/\partial x]\, u_x = a^{1/2}\, u_x$,
- Hence, $v_{xx} = a^{1/2}\, a^{1/2}\, u_{xx} = a\, u_{xx}$.

Note that the particular initial condition $Q(x, 0)$ does not change under dilation.

We will find $Q(x, t)$ in three steps then, the 4th step will provide us with $u(x, t)$

① We look for $Q(x, t)$ of a particular form, inspired from the invariance properties of the diffusion equation.

② Based on this particular form for $Q(x, t)$, we convert the diffusion equation into an ODE, which we easily solve.

③ We set the value of integration constants by *carefully* applying the particular initial condition $Q(x, 0)$, ending up with a fully explicit formula for $Q(x, t)$.

④ After, we will find $u(x, t)$ for a general IC.

We look for $Q(x, t)$ of a particular form

① We look for $Q(x, t)$ of the form

$$Q(x,t) = g(p) \quad \text{where } p = \frac{x}{\sqrt{4kt}}$$

and g is an unknown function of only one variable.

❺ If $u(x, t)$ is a solution, so is the dilated function

$u(a^{1/2}x, a\, t)$, for any $a > 0$.

The factor 4 k is included only to facilitate later simplifications.

We expect Q to have this special form because it is supposed to remain unchanged under dilation

Both the diffusion equation and the considered IC do not change under the dilation

$$x \longrightarrow a^{1/2}\, x \qquad \text{and} \qquad t \longrightarrow a\, t\,.$$

Therefore, $Q(x, t)$ <u>must</u> also remain unchanged under this dilation.

How could that happen?

In only one way: if Q depends on x and t solely through the combination $x\,/\,t^{1/2}$, since the dilation takes $x\,/\,t^{1/2}$ into $a^{1/2}x/(at)^{1/2} = x\,/\,t^{1/2}$.

Thus let $p = x\,/\,(4kt)^{1/2}$ and look for $Q = g(p)$ …

We convert the diffusion equation into an ODE

② Applying the chain rule with

$$Q(x,t) = g(p) \quad \text{where } p = \frac{x}{\sqrt{4kt}}$$

leads to

$$Q_t = \frac{dg}{dp}\frac{\partial p}{\partial t} = -\frac{1}{2t}\frac{x}{\sqrt{4kt}}g'(p)$$

$$Q_x = \frac{dg}{dp}\frac{\partial p}{\partial x} = \frac{1}{\sqrt{4kt}}g'(p)$$

$$Q_{xx} = \frac{dQ_x}{dp}\frac{\partial p}{\partial x} = \frac{1}{4kt}g''(p)$$

We convert the diffusion equation into an ODE

Substituting

$$Q_t = \frac{dg}{dp}\frac{\partial p}{\partial t} = -\frac{1}{2t}\frac{x}{\sqrt{4kt}}g'(p)$$

and

$$Q_{xx} = \frac{dQ_x}{dp}\frac{\partial p}{\partial x} = \frac{1}{4kt}g''(p)$$

into the diffusion equation leads to

$$0 = Q_t - kQ_{xx} = \frac{1}{t}\left[-\frac{1}{2}pg'(p) - \frac{1}{4}g''(p)\right]$$

Consequently: $\quad g'' + 2pg' = 0$

The obtained ODE is easily solved

Setting $f = g'$, the ODE $\quad g'' + 2pg' = 0$

becomes $f' + 2pf = 0$, hence:

$$g'(p) = c_1 \exp(-p^2)$$

and $\quad Q(x,t) = c_1 \int_0^{x/\sqrt{4kt}} e^{-p^2} dp + c_2$

which is valid <u>only</u> for $t > 0$!!!

Therefore, care must be taken when applying the IC …

To find a completely explicit formula for $Q(x, t)$, the particular initial condition is applied using limits

③ If $x > 0$,

see Gaussian integrals

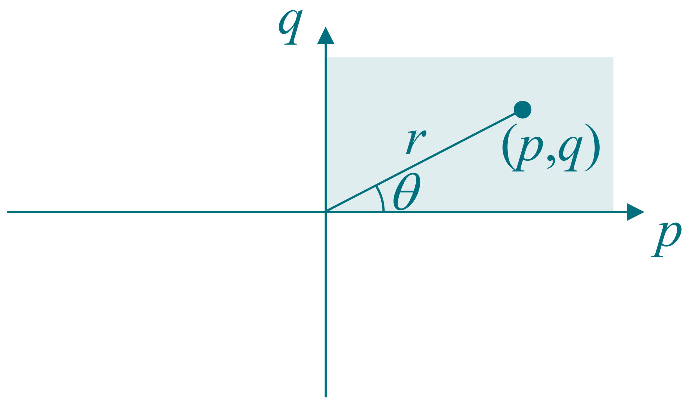
$$1 = \lim_{t \searrow 0} Q = c_1 \int_0^{+\infty} e^{-p^2}\,dp + c_2 = c_1 \frac{\sqrt{\pi}}{2} + c_2$$

If $x < 0$,

$$0 = \lim_{t \searrow 0} Q = c_1 \int_0^{-\infty} e^{-p^2}\,dp + c_2 = -c_1 \frac{\sqrt{\pi}}{2} + c_2$$

$$Q(x,t) = c_1 \int_0^{x/\sqrt{4kt}} e^{-p^2}\,dp + c_2$$

Gaussian integral



Our goal is to evaluate this number:

$$I = \int_0^{\infty} e^{-p^2}\, dp = {\color{red}-}\int_0^{-\infty} e^{-p^2}\, dp$$

It turns out to be easier to evaluate the square of I:

$$I^2 = \int_0^{\infty} e^{-p^2}\, dp \int_0^{\infty} e^{-q^2}\, dq = \int_0^{\infty}\int_0^{\infty} e^{-\left(p^2+q^2\right)}\, dp\, dq$$

Change variables and use polar coordinates:

$$I^2 = \int_0^{\pi/2}\int_0^{\infty} r\, e^{-r^2}\, dr\, d\theta = \frac{\pi}{2}\left[-\frac{1}{2}e^{-r^2}\right]_0^{\infty} = \frac{\pi}{4} \Rightarrow \boxed{I = \frac{\sqrt{\pi}}{2}}$$

To find a completely explicit formula for $Q(x, t)$, the particular initial condition is applied using limits

③ If $x > 0$,

see Gaussian integrals

$$1 = \lim_{t \searrow 0} Q = c_1 \int_0^{+\infty} e^{-p^2} dp + c_2 = c_1 \frac{\sqrt{\pi}}{2} + c_2$$

If $x < 0$,

$$0 = \lim_{t \searrow 0} Q = c_1 \int_0^{-\infty} e^{-p^2} dp + c_2 = -c_1 \frac{\sqrt{\pi}}{2} + c_2$$

This determines the coefficients c_1 and c_2 and leads to the following expression for Q, valid for $t > 0$:

You may check that $Q(x, t)$ satisfies the diffusion equation!

$$Q(x, t) = \frac{1}{2} + \frac{1}{\sqrt{\pi}} \int_0^{x/\sqrt{4kt}} e^{-p^2} dp$$

The solution of diffusion problems is sometimes expressed in terms of the *error function* of statistics

Expression

$$Q(x,t) = \frac{1}{2} + \frac{1}{\sqrt{\pi}} \int_0^{x/\sqrt{4kt}} e^{-p^2}\, dp$$

may be expressed as

$$Q(x,\ t) = \frac{1}{2} + \frac{1}{2}\mathscr{E}\mathrm{rf}\left(\frac{x}{\sqrt{4kt}}\right)$$

where the *error function* has been introduced:

$$\mathscr{E}\mathrm{rf}(x) = \frac{2}{\sqrt{\pi}} \int_0^{x} e^{-p^2}\, dp$$

From $Q(x, t)$, let us build the general solution $u(x, t)$ valid for an arbitrary initial condition $\phi(x)$

④ We claim that the general (and unique) solution of the *diffusion problem* writes, for $t > 0$:

$$u(x, t) = \int_{-\infty}^{\infty} S(x - y, t)\phi(y)\, dy$$

with $S = \partial Q \,/\, \partial x$.

Now, we need to prove that:

- $u(x, t)$ is indeed a solution of the diffusion equ.
- $u(x, t)$ satisfies the general initial condition $\phi(x)$

$u(x, t)$ is indeed a solution of the diffusion equation

We claim that the general (and unique) solution of the *diffusion problem* writes, for $t > 0$:

$$u(x, t) = \int_{-\infty}^{\infty} S(x - y, t)\phi(y)\, dy$$

with $S = \partial Q / \partial x$.

- From invariance property ❷, $S = \partial Q / \partial x$ is also a solution of the diffusion equation

- From invariance property ❹, $u(x, t)$ is also a solution of the diffusion equation

$u(x, t)$ satisfies the general initial condition $\phi(x)$

Demonstrating that $u(x, t)$ satisfies the general initial condition $\phi(x)$ requires some calculation.

$$u(x,t) = \int_{-\infty}^{\infty} \frac{\partial Q}{\partial x}(x-y,t)\phi(y)\,dy$$

This integration by parts enables overcoming the discontinuity in $Q(x,0)$!

$$= -\int_{-\infty}^{\infty} \frac{\partial}{\partial y}[Q(x-y,t)]\phi(y)\,dy$$

$$= +\int_{-\infty}^{\infty} Q(x-y,t)\phi'(y)\,dy - Q(x-y,t)\phi(y)\Big|_{y=-\infty}^{y=+\infty}$$

The limits vanish if we assume that $\phi(y)$ equals zero for $|y|$ large.

$u(x, t)$ satisfies the general initial condition $\phi(x)$

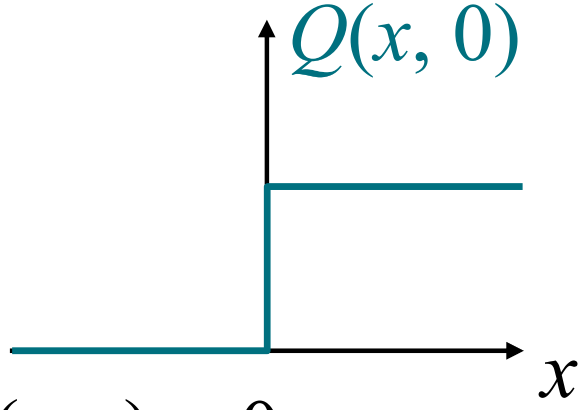
Therefore,

$$u(x, 0^+) = \int_{-\infty}^{\infty} Q(x - y, 0^+)\phi'(y)\, dy$$

$$= \int_{-\infty}^{x} \phi'(y)\, dy = \phi\Big|_{-\infty}^{x} = \phi(x)$$

because of

- the initial condition for Q
- and the assumption that $\phi(-\infty) = 0$



As a conclusion, we have now an explicit formula for the solution of the *diffusion problem*

The solution writes

$$u(x,t) = \int_{-\infty}^{\infty} S(x-y,t)\phi(y)\,dy$$

with, for $t > 0$,

$$S = \frac{\partial Q}{\partial x} = \frac{1}{2\sqrt{\pi k t}} e^{-x^2/4kt}$$

Hence,

$$\boxed{u(x,t) = \frac{1}{\sqrt{4\pi k t}} \int_{-\infty}^{\infty} e^{-(x-y)^2/4kt} \phi(y)\,dy}$$

2 – Green’s function

In this section, we highlight the concept and properties of Green’s function, which is found to be the fundamental solution of the diffusion equation

Concept of *source function*, or *Green's function*, or *fundamental solution* of the diffusion problem

In the solution

$$u(x,t) = \boxed{\frac{1}{\sqrt{4\pi kt}}} \int_{-\infty}^{\infty} \boxed{e^{-(x-y)^2/4kt}} \phi(y)\, dy$$

$$S(x,t) = \frac{1}{2\sqrt{\pi kt}} e^{-x^2/4kt}$$

$S(x, t)$ is known as

- the source function,
- Green's function,
- fundamental solution,
- Gaussian,
- or propagator of the diffusion equation,
- or the diffusion kernel.

The solution formula for the diffusion equation is an example of a convolution

$$S(x,t) = \frac{1}{2\sqrt{\pi k t}} e^{-x^2/4kt}$$

The solution

$$u(x,t) = \int_{-\infty}^{\infty} \boxed{S(x-y,t)}\,\phi(y)\,dy = \int_{-\infty}^{\infty} \boxed{S(z,t)}\,\phi(x-z)\,dz$$

is the convolution of ϕ with S (at a fixed t).

Indeed, if $f(x)$ and $g(x)$ are two functions of a real variable, their convolution (noted $f * g$) is defined as:

$$(f * g)(x) = \int_{-\infty}^{\infty} f(x-y)g(y)\,dy$$

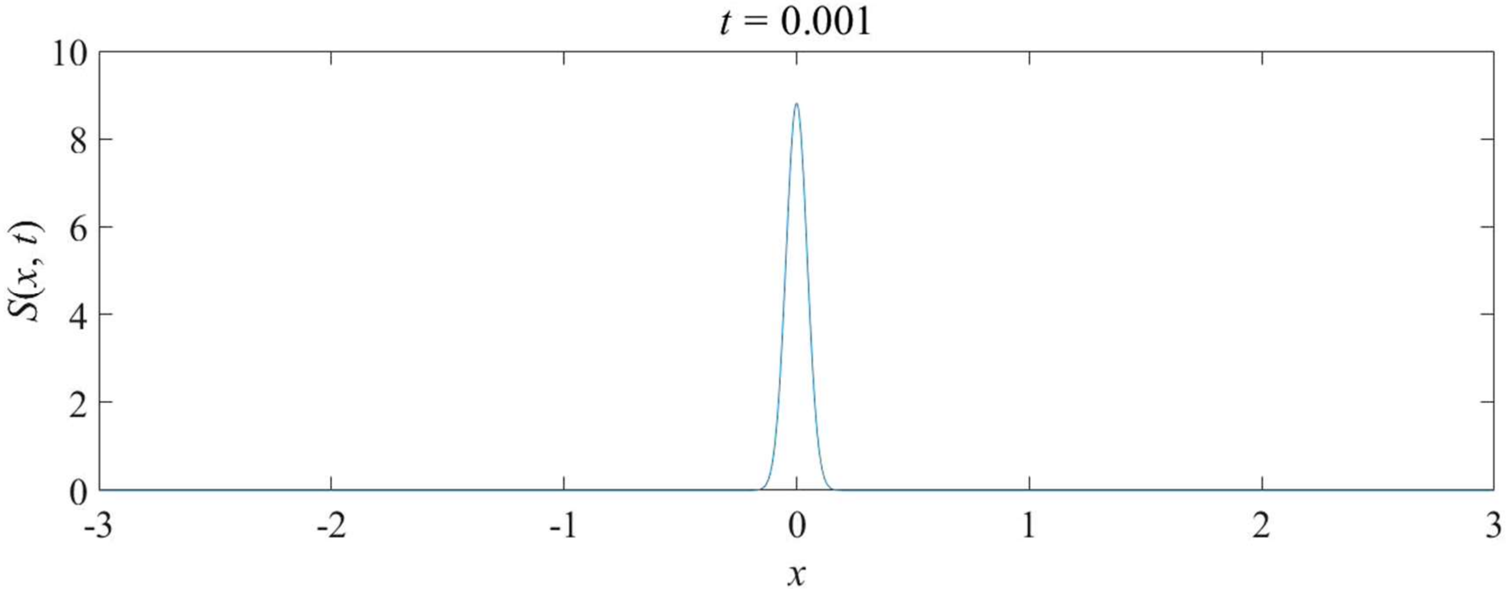
Convolution plays a central role in probability theory and it shows interesting properties in relationship with Fourier transform. See a next lecture.

Properties of the *source function*

The source function

$$S(x,t) = \frac{1}{2\sqrt{\pi k t}} e^{-x^2/4kt}$$

- is defined for all real x and for all $t > 0$
- is even in x, i.e. $S(-x, t) = S(x, t)$



Properties of the *source function*

- The integral of the source function is 1:

$$\int_{-\infty}^{\infty} S(x,t)\,dx = \frac{1}{2\sqrt{\pi kt}} \int_{-\infty}^{\infty} e^{-x^2/4kt}\,dx$$

$$= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-p^2}\,dp = 1$$

- For a very small t, the function $S(x, t)$ takes very small values everywhere except for a tall spike:

$$\max_{|x|>\delta} S(x,t) \to 0 \quad \text{for} \quad t \to 0$$

Physical interpretation

Notice that the value of the solution $u(x, t)$

$$u(x,t) = \int_{-\infty}^{\infty} S(x-y,t)\,\phi(y)\,dy$$

is a kind of weighted average of the initial values around the point x. Indeed, we can write

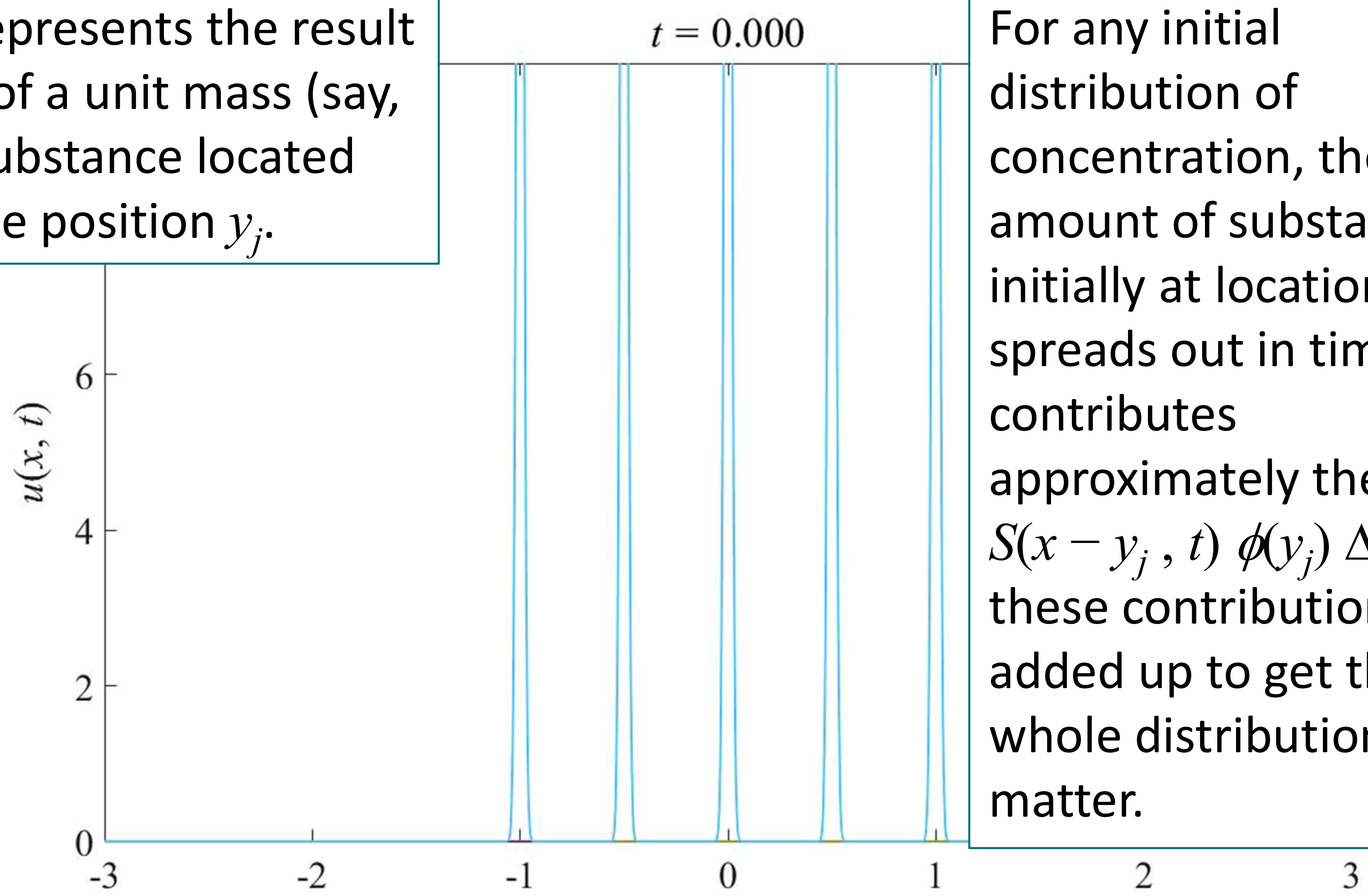
$$u(x,t) \simeq \sum_j \underbrace{S(x-y_j,t)}_{\text{weights}}\,\phi(y_j)\,\Delta y_j$$

- For very small t, the source function is a spike so that the formula "overweights" the values of ϕ near x.
- For any $t > 0$ the solution is a spread-out version of the initial values at $t = 0$.

Physical interpretation: $u(x,t) \simeq \sum_j S(x - y_j, t)\,\phi(y_j)\,\Delta y_j$

weights

$S(x - y_j,\, t)$ represents the result of diffusion of a unit mass (say, 1 gram) of substance located initially at the position y_j.



For any initial distribution of concentration, the amount of substance initially at locations y_j spreads out in time and contributes approximately the term $S(x - y_j\,,\, t)\ \phi(y_j)\ \Delta y_j$. All these contributions are added up to get the whole distribution of matter.

$S(x - y_j,\, t)$ may also represent the result of a “hot spot” at y_j at time 0. The hot spot is cooling off and spreading its heat along the rod.

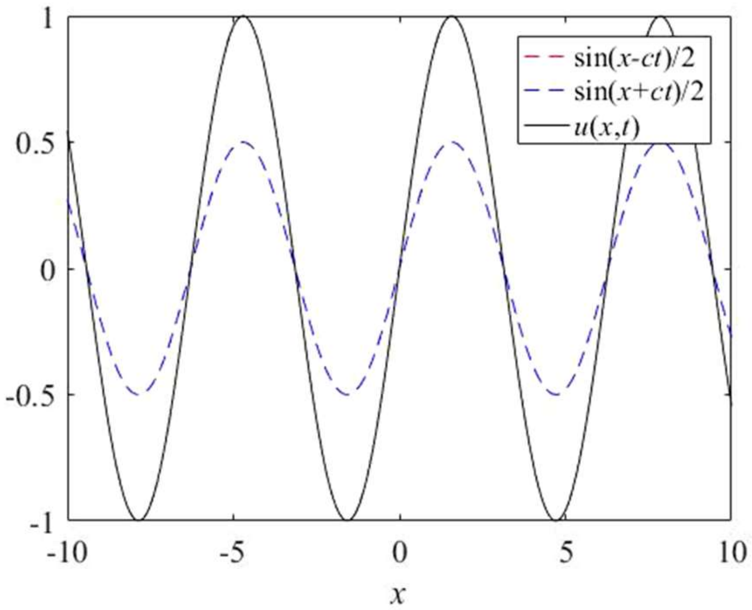
3 – Comparison of waves and diffusions

In this section, we emphasize the contrasting basic properties of the wave equation and the diffusion equation (Section 2.5 in Strauss, 2008).

The basic properties of waves and diffusions differ substantially

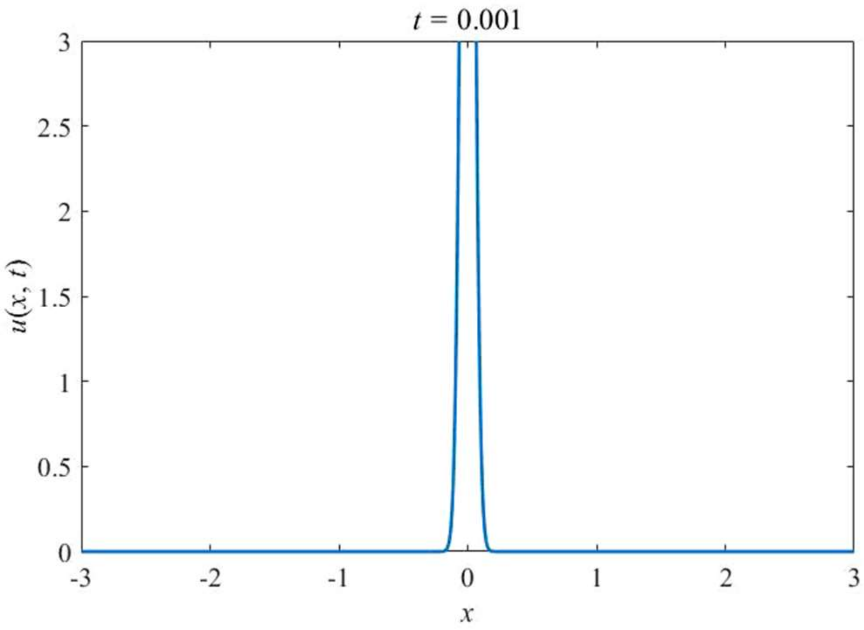
Wave equation

Information gets transported in both directions at a finite speed.



Diffusion equation

The initial disturbance gets spread out in a smooth fashion and gradually disappears.



In contrast with waves, the speed of propagation is infinite in diffusions

In diffusions, the value of $u(x, t)$ depends on the values of the IC $\phi(y)$ for all y, where $-\infty < y < \infty$:

$$u(x,t) = \frac{1}{\sqrt{4\pi kt}} \int_{-\infty}^{\infty} e^{-(x-y)^2/4kt} \phi(y)\, dy$$

Conversely, the value of ϕ at a point x_0 has an immediate effect everywhere (for $t > 0$), even though most of its effect is only near x_0.

This contrasts with the solution of wave problems:

$$u(x,t) = \frac{1}{2}[\phi(\boxed{x+ct}) + \phi(\boxed{x-ct})] + \frac{1}{2c}\int_{x-ct}^{x+ct} \psi(s)\, ds.$$

Take-home messages

Property		Waves	Diffusions
(i)	Speed of propagation?	Finite ($\leq c$)	Infinite
(ii)	Singularities for $t > 0$?	Transported along characteristics (speed $= c$)	Lost immediately
(iii)	Well-posed for $t > 0$?	Yes	Yes (at least for bounded solutions)
(iv)	Well-posed for $t < 0$?	Yes	No
(v)	Maximum principle	No	Yes
(vi)	Behavior as $t \to +\infty$?	Energy is constant so does not decay	Decays to zero (if ϕ integrable)
(vii)	Information	Transported	Lost gradually

The diffusion equation describes physical processes such as heat flow, Brownian motion, … that are irreversible.