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)

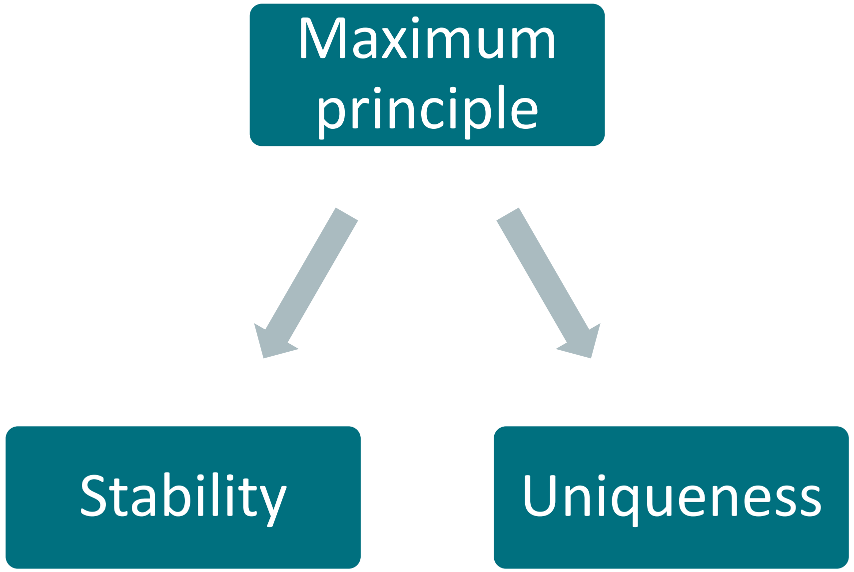
3. Concept and properties of Green's function,
or fundamental solution of the diffusion equation

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

# Reminder

We study the 1D diffusion equation:

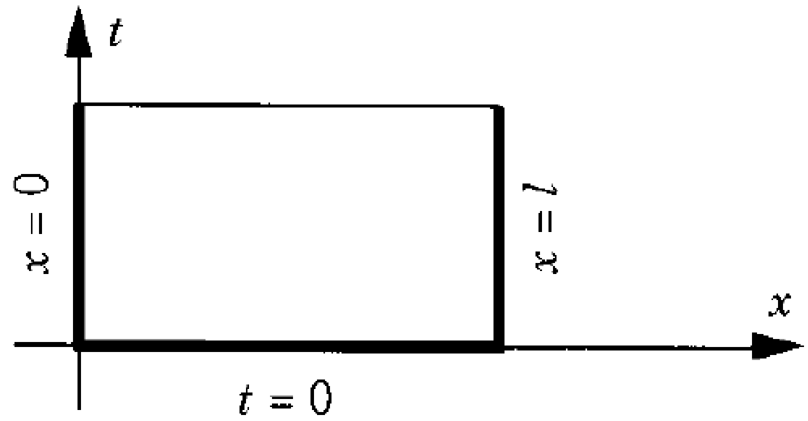
$$u_t = k u_{xx}$$



# Maximum principle

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 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. ↗



# 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

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

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

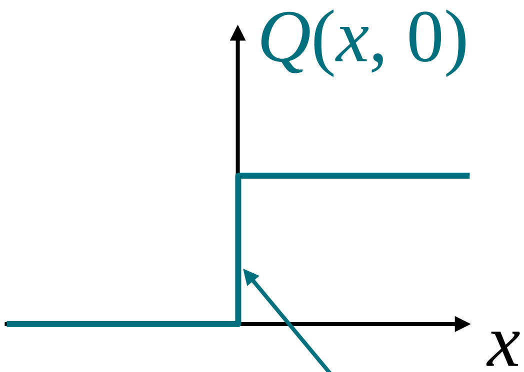
① • to solve it for a particular *initial condition* $\phi(x)$

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

➊ 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 $v_t = k\, v_{xx}$

➋ 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

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

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, $Q(x, t)$ must 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: $g'' + 2pg' = 0$

# The obtained ODE is easily solved

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

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

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

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

which is valid only 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*

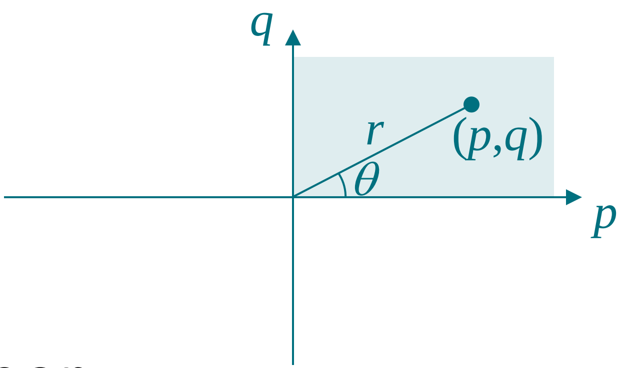
$$1 = \lim_{t \searrow 0} Q = c_1 \int_0^{+\infty} e^{-p^2} dp + c_2 = c_1 \frac{\sqrt{\pi}}{2} + c_2$$

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:

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

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:

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

# 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 $t > 0$:

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

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

# 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.

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

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

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

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

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

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

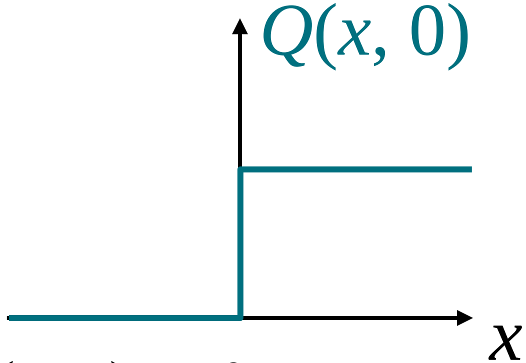
Therefore,

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

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

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,

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

# Reminder: Leibniz integral rule

For sufficiently continuous functions $f(x,t)$, $a(x)$ and $b(x)$,

$$\frac{d}{dx}\left(\int_{a(x)}^{b(x)} f(x,t)\ dt\right) = f\left(x, b(x)\right)\frac{d}{dx}b(x) - f\left(x, a(x)\right)\frac{d}{dx}a(x) + \int_{a(x)}^{b(x)} \frac{\partial f}{\partial x}(x,t)\ dt$$

# 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

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

is the convolution of $\phi$ 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:

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

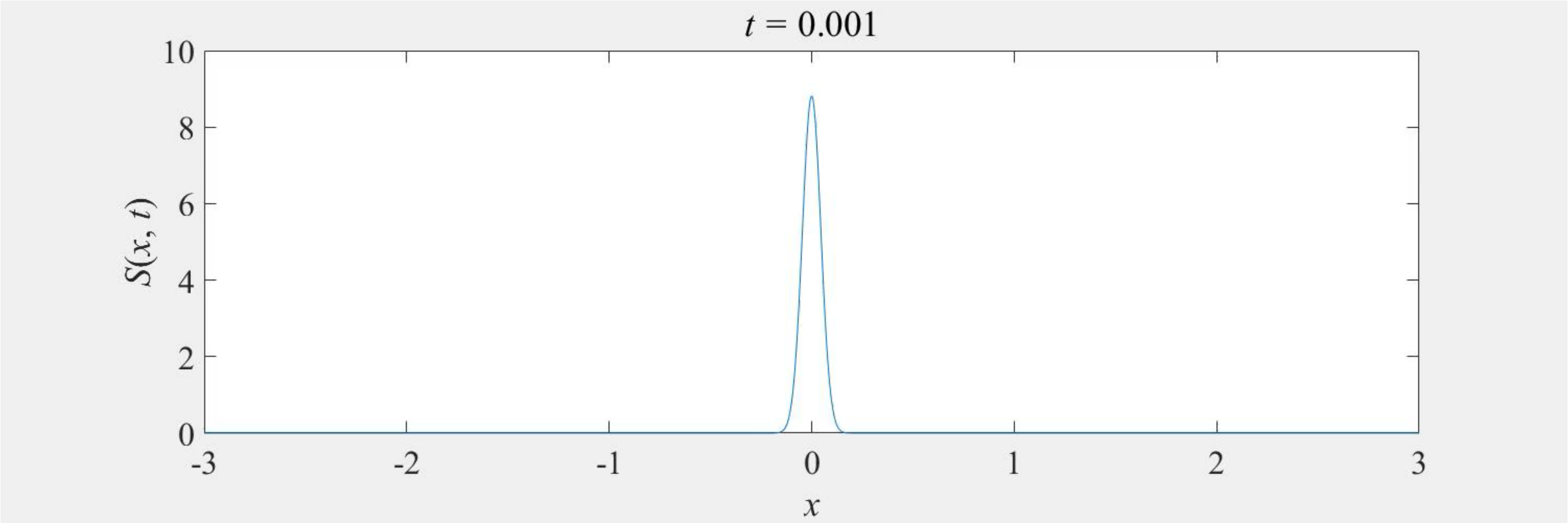
Convolution plays a central role in probability theory and it shows interesting properties in relation to Fourier transform. See upcoming lecture.

# 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:

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

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

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

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

# 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

$$u(x,t)\simeq\sum_{j} S(x-y_j,t)\,\phi(y_j)\,\Delta y_j$$

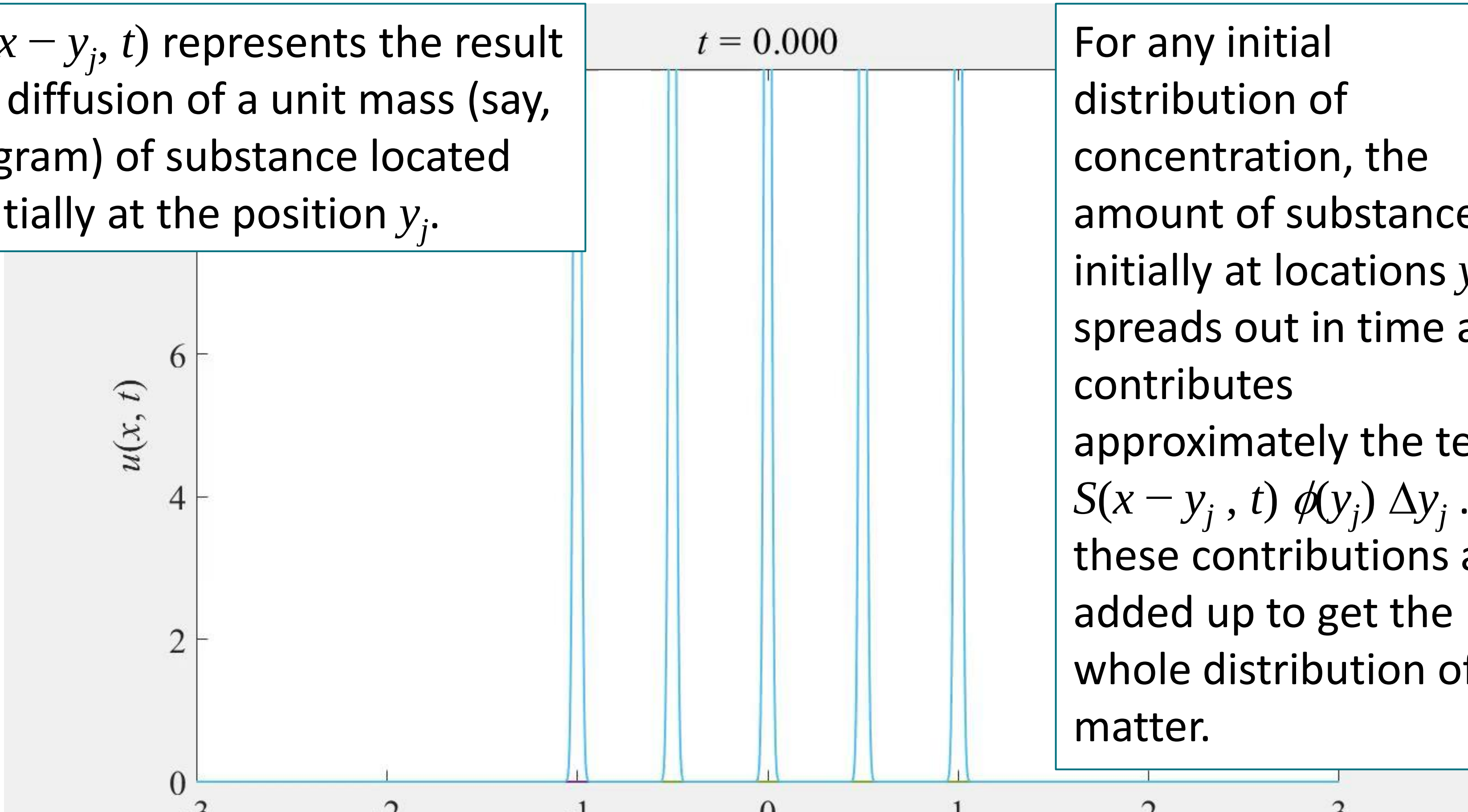
↑ weights

- For very small $t$, the source function is a spike so that the formula "overweights" the values of $\phi$ 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.

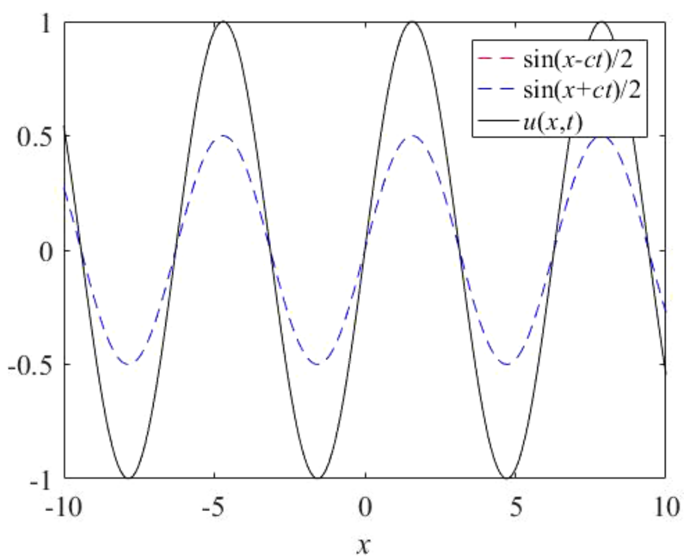
# 3 – Comparison of waves and diffusions

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

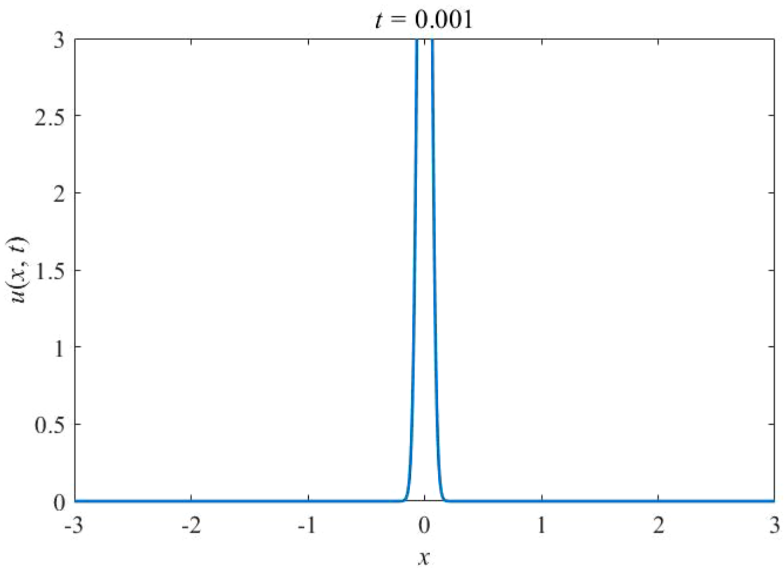
**Wave equation**

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 $-\infty < y < \infty$:

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

The value of $\phi$ 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:

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

# 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 $\phi$ integrable) |
| (vii) | Information | Transported | Lost gradually |

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