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Applied Differential Calculus

LECTURE 5: Fourier series and separation of variables: Heat equation.

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I. INTRODUCTION: CLASSIFICATION OF SECOND-ORDER PDES

Linear second order PDEs very often describe many phenomena in Engineering. Among them, the **heat equation** (**parabolic PDE**), the **wave equation** (**hyperbolic PDE**) and the **Laplace equation** (**elliptic PDE**) have paramount importance as they are paradigms of phenomena occurring in many different fields.

Given a **general linear second-order PDE with constant coefficients**, a_{ij}, b_i, c,

$$\sum_{i,j=1}^{2} a_{ij}\partial_{x_i}\partial_{x_j}u + \sum_i b_i\partial_{x_i}u + cu = F(x,y), \tag{1}$$

we would like to know which initial and/or boundary values would render the **solution** $u(x,y)$ (with $x_1 = x$, $x_2 = y$) **unique**.

We can always select a_{ij} so that $a_{ij} = a_{ji}$.

The first idea could be to **change variables** in (1) so that this PDE acquires some **canonical form**.

Let

$$x_i = \sum_{j=1}^{2} R_{ij}\xi_j, \quad \xi_i = \sum_{j=1}^{2} R^{-1}_{ij}x_j, \tag{2}$$

change variables from (x_1, x_2) to ξ_1, ξ_2 (with $\xi_1 = \xi$, $\xi_2 = \eta$).

Inserting (2) into (1), we find

$$\sum_{i,j,k,l=1}^{2} a_{ij}R^{-1}_{ki}R^{-1}_{lj}\partial_{\xi_k}\partial_{\xi_l}u + \sum_{i,k=1}^{2} b_iR^{-1}_{ki}\partial_{\xi_k}u + cu = F. \tag{3}$$

Since the matrix of coefficients a_{ij} is symmetric, it has real eigenvalues λ_i and it can be diagonalized by an orthogonal matrix $\underline{\underline{R}}^{-1} = \underline{\underline{R}}^T$.

Selecting this matrix for the change of variable (2),

$$\sum_{i,j,=1}^{2} a_{ij}R^{-1}_{ki}R^{-1}_{lj} = \left(\underline{\underline{R}}^{-1}\underline{\underline{A}}(\underline{\underline{R}}^{-1})^T\right)_{kl} = \left(\underline{\underline{R}}^{-1}\underline{\underline{A}}\,\underline{\underline{R}}\right)_{kl} = \lambda_k\delta_{kl}.$$

Then (1) becomes

$$\sum_{k=1}^{2} \lambda_k\partial^2_{\xi_k}u + \sum_i b_iR_{ik}\partial_{\xi_k}u + cu = F. \tag{4}$$

Depending on the eigenvalues, we have the following **cases**:

i) **Case det$\underline{\underline{A}} = a_{11}a_{22} - a_{12}^2 < 0$, then $\lambda_1\lambda_2 =$ det$\underline{\underline{A}} < 0$, so that $\lambda_1 < 0 < \lambda_2$.**

The PDE is called ***hyperbolic***.

Rescaling $\Xi_1 = |\lambda_1|^{-1/2}\xi_1$ and $\Xi_2 = \lambda_2^{-1/2}\xi_2$, this PDE can be written as

$$-\partial^2_{\Xi_1} u + \partial^2_{\Xi_2} u = \ldots, \qquad (5)$$

where we have omitted all terms with first-order or no derivatives.

The **wave equation** is a typical **hyperbolic PDE** and initial (**two initial conditions**) and **boundary conditions** can be imposed to obtain a **unique solution**.

ii) **Case det$\underline{\underline{A}} = \lambda_1\lambda_2 > 0$.**

The two eigenvalues are both positive or both negative.

The PDE is called ***elliptic***.

Rescaling $\Xi_1 = |\lambda_1|^{-1/2}\xi_1$ and $\Xi_2 = |\lambda_2|^{-1/2}\xi_2$, this PDE can be written as

$$\partial^2_{\Xi_1} u + \partial^2_{\Xi_2} u = \ldots. \qquad (6)$$

The **Laplace equation** and the **Poisson equation** are typical **elliptic equations**. **Only boundary conditions** can be imposed on these equations to obtain a **unique solution**.

iii) **Case the determinant of the coefficient matrix is zero and therefore one eigenvalue is zero**.

For instance, $\lambda_1 = 0$. Then the PDE is called ***parabolic***.

Rescaling $\Xi_2 = \lambda_2^{-1/2}\xi_2$, this PDE can be written as

$$\partial^2_{\Xi_2} u = \ldots. \qquad (7)$$

The **heat equation** is a typical **parabolic PDE** and **boundary conditions** and **one initial condition** (there is only one derivative with respect to ξ_1) can be imposed to obtain a **unique solution**.

A similar classification can be found when u depends on more than two variables.
For n independent variables, **hyperbolic equations** correspond to a coefficient matrix having $(n-1)$ positive (resp. negative) eigenvalues and one negative (resp. positive) eigenvalue. **Elliptic equations** are obtained when all the eigenvalues are non zero and have the

same sign. **Parabolic equations** have $(n-1)$ eigenvalues of the same sign and one zero eigenvalue.

Example 1.

Let us classify the equation

$$\partial_x^2 u + 2\partial_x \partial_y u - \partial_y^2 u = \partial_x u + 1.$$

The coefficient matrix has components $a_{11} = 1$, $a_{12} = a_{21} = 1$, $a_{22} = -1$, with negative determinant -2. One eigenvalue is positive, the other negative. In fact, the eigenvalue equation is $\lambda^2 - 2 = 0$. Then $\lambda = \pm\sqrt{2}$ and the equation is **hyperbolic**.

A similar classification can be made for equations with **variable coefficients**. The changes of variable lead to more complicated formulas but if we only keep track of the second derivatives of u, the first term of (3) is still the same and we can diagonalize the coefficient matrix in the same way. The difference now is that the eigenvalues will be non-constant functions.

Example 2.

Let us classify the **Tricomi equation**

$$\partial_y^2 u - y\partial_x^2 u = 0.$$

The coefficient matrix has components $a_{11} = -y$, $a_{12} = 0$, $a_{22} = 1$. The determinant of the coefficient matrix is $-y$ and therefore the Tricomi equation is **hyperbolic** for $y > 0$, **elliptic** for $y < 0$ and **parabolic** for $y = 0$.

II. HEAT EQUATION

We start by studying **heat conduction in solid bodies**.

The rate of change of internal energy density in a spatial region R (that does not change with time) in three-dimensional space equals the heat energy flowing across the boundaries ∂R per unit time plus the heat energy per unit time $\int_R Q(\underline{x}, t)\, dV$ produced by internal sources.

The internal energy is the volume integral over R of the mass density ρ times the specific heat c times the temperature $u(\underline{x}, t)$.

The heat energy flowing out of the region R per unit time per unit surface area is the outward normal component of the heat flux: $\underline{q}\cdot\underline{n}$, where $\underline{n}$ is the unit outward normal vector: $\underline{q}\cdot\underline{n} > 0$ means that the heat is leaving the region R, whereas if $\underline{q}\cdot\underline{n} < 0$ the heat is flowing to R. Then conservation of energy yields

$$\frac{d}{dt}\int_R \rho c u \, dV = -\oint_{\partial R} \underline{q}\cdot\underline{n}\, dS + \int_R Q(\underline{x},t)\, dV. \tag{8}$$

The divergence theorem says that $\oint_{\partial R} \underline{q}\cdot\underline{n}\, dS = \int_R \nabla\cdot\underline{q}\, dV$ which, inserted in (8), produces

$$\int_R \left(\rho c\frac{\partial u}{\partial t} + \nabla\cdot\underline{q} - Q(\underline{x},t)\right) dV = 0. \tag{9}$$

Here we have assumed that ρ and c are time-independent and that R is any arbitrary fixed region.

Assuming also that the integrand in Eq. (9) is continuous, it must be zero. This yields

$$\rho c\frac{\partial u}{\partial t} = -\nabla\cdot\underline{q} + Q(\underline{x},t). \tag{10}$$

Experiments indicate that heat flows from hot to cold bodies in contact trying to equate their temperatures.

This is expressed by **Fourier's law** relating the heat flux to the gradient of temperature

$$\underline{q} = -K\nabla u. \tag{11}$$

K is the **thermal conductivity**.

Fourier's law is a constitutive relation between $\underline{q}$ and u. Substituting (11) into (10), we obtain the partial differential equation (PDE) for the **unknown temperature** $u(\underline{x},t)$:

$$\rho c\frac{\partial u}{\partial t} = \nabla\cdot(K\nabla u) + Q(\underline{x},t), \tag{12}$$

in which ρ, c, K and Q are supposed to be known functions.

If ρ, c and K are constant, we can rewrite (12) as

$$\frac{\partial u}{\partial t} = k\nabla^2 u + f(\underline{x},t), \tag{13}$$

where the $k = K/(\rho c)$ is the **thermal diffusivity** and $f = Q/(\rho c)$ has units of temperature per unit time.

If the body is a slender rod directed along the x axis, (13) becomes **the one-dimensional heat equation**:

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} + f(x,t).$$

This equation has **two derivatives in space** and **one in time** so that we need to specify one initial conditions and boundary conditions at two different points to expect a **unique solution**.

For example, if we specify the temperature at the two ends of the rod to be zero and the initial temperature to be $u_0(x)$, we obtain the following initial-boundary value problem (IBVP):

$$\begin{aligned}\frac{\partial u}{\partial t} - k\frac{\partial^2 u}{\partial x^2} &= f(x,t), \quad 0 < x < l, \quad t > t_0, \qquad (14)\\ u(x,t_0) &= u_0(x), \quad 0 < x < l,\\ u(0,t) &= 0, \quad t > t_0,\\ u(l,t) &= 0, \quad t > t_0.\end{aligned}$$

Zero values of the unknown at the boundaries give rise to a so-called **homogeneous *Dirichlet problem*** (non-zero values of the temperature at the ends of the rod constitute a **inhomogeneous Dirichlet problem**).

Of course we could have selected two nonzero temperatures at the ends of the rod, for example $u(0,t) = T_0$ and $u(l,t) = T_l$.

But the change $u(x,t) = T_0 + (T_l - T_0)x/l + v(x,t)$ produces the same equation (14) for v and now $v = 0$ at both $x = 0, l$.

There are other reasonable boundary conditions: fixed heat flux at the ends or **Newton's law of cooling**.

For instance, insulated ends mean that the heat flux is zero in them. Then **Fourier's law** says that we have to replace the boundary conditions by

$$\begin{aligned}\frac{\partial u}{\partial x}(0,t) &= 0, \quad t > t_0,\\ \frac{\partial u}{\partial x}(l,t) &= 0, \quad t > t_0. \qquad (15)\end{aligned}$$

These conditions are known as zero-flux or **homogeneous *Neumann boundary conditions*** (non-zero values of the heat flux at the ends of the rod constitute a inhomogeneous Neumann problem).

Lastly, if the rod ends are open in a room at a lower temperature than the rod, the heat flows from the rod towards the room at a rate that is proportional to the difference of temperature with the room (**Newton's law of cooling**).

The resulting boundary conditions are

$$\begin{aligned} \frac{\partial u}{\partial x}(0,t) &= -h[u(0,t)-u_r], \quad t>t_0, \\ \frac{\partial u}{\partial x}(l,t) &= h[u(l,t)-u_r], \quad t>t_0, \end{aligned} \tag{16}$$

which are called **inhomogeneous *Robin*** (or **mixed**) boundary conditions.
If $u_r = 0$, we have homogeneous Robin boundary conditions.

A. Fourier series method for the heat equation

1. *Separation of variables for the homogeneous heat equation*

We start by trying to solve the homogeneous heat equation (14) with $f = 0$.
To this end, we look for special solutions of the form

$$u_p(x,t) = X(x)T(t), \tag{17}$$

that are products of functions of x and functions of t. We insert (17) into the homogeneous heat equation

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} \Longrightarrow T'(t)X(x) = T(t)X''(x),$$

and divide the result by u_p, thereby obtaining

$$\frac{T'(t)}{k\,T(t)} = \frac{X''(x)}{X(x)}. \tag{18}$$

The left hand side of this equation is a function of t and the right hand side is a function of x. Then both sides are equal to a constant (because taking an x derivative of the equation, the left hand side gives zero and therefore the x derivative of $\frac{X''(x)}{X(x)}$ is zero, therefore yielding $\frac{X''(x)}{X(x)} = -\lambda$, a constant).
Then we get

$$X''(x) + \lambda X(x) = 0, \quad T'(t) = -\lambda k\,T(t). \tag{19}$$

λ is called the ***separation constant***.

2. ***Eigenvalue problem for*** $X(x)$

The Dirichlet boundary conditions yield $X(0) = 0$ and $X(l) = 0$, so that the spatial function $X(x)$ satisfies the BVP:

$$X''(x) + \lambda X(x) = 0, \quad 0 < x < l, \tag{20}$$
$$X(0) = 0, \quad X(l) = 0.$$

Obviously $X(x) = 0$ is a solution of (20), but we are interested in knowing whether (20) has nonzero solutions for some particular value of λ.
This is a typical ***eigenvalue problem***: its nonzero solutions are called ***eigenfunctions*** and the corresponding separation constants λ are the **eigenvalues**.
Assuming $\lambda > 0$, (20) has the general solution

$$X(x) = c_1 \cos(\sqrt{\lambda} x) + c_2 \sin(\sqrt{\lambda} x).$$

Substituting this into the first boundary condition, we get $0 = X(0) = c_1$. Then we find $X(x) = c_2 \sin(\sqrt{\lambda} x)$ and the second boundary condition yields

$$c_2 \sin(l\sqrt{\lambda}) = 0 \Longrightarrow l\sqrt{\lambda} = n\pi, \quad n = 1, 2, \ldots. \tag{21}$$

We have found the following pairs of eigenvalues and eigenfunctions for (20):

$$\lambda_n = \frac{n^2\pi^2}{l^2}, \quad X_n(x) = \sin\frac{n\pi x}{l}, \quad n = 1, 2, \ldots. \tag{22}$$

For each of these eigenvalues, the solution of the ODE for T in (19) is

$$T_n(t) = e^{-n^2\pi^2 kt/l^2}. \tag{23}$$

Are there any other eigenfunctions?
You can check that the only solution (20) has for $\lambda \leq 0$ is $X(x) = 0$.
Now that we have found infinitely many particular solutions of the homogeneous heat equation with Dirichlet boundary conditions, we use the **superposition principle** to say that

$$u(x,t) = \sum_{n=1}^{\infty} a_n e^{-n^2\pi^2 kt/l^2} \sin\frac{n\pi x}{l}, \tag{24}$$

with constant coefficients a_n is a solution of the heat equation (whenever this series converges) that satisfies the Dirichlet boundary conditions.

To calculate the **coefficients** a_n, we use the initial condition in (20)

$$u_0(x) = u(x,0) = \sum_{n=1}^{\infty} a_n \sin\frac{n\pi x}{l}. \tag{25}$$

Using the **trigonometric integrals**:

$$\int_0^l \sin\frac{n\pi x}{l}\sin\frac{m\pi x}{l} dx = \frac{1}{2}\int_0^l \left[\cos\frac{(m-n)\pi x}{l} - \cos\frac{(m+n)\pi x}{l}\right] dx$$

$$= \frac{1}{2}\left[\frac{\sin[(m-n)\pi x/l]}{(m-n)\pi} - \frac{\sin[(m+n)\pi x/l]}{(m+n)\pi}\right]\Bigg|_0^l = \frac{l}{2}\delta_{mn} = \frac{l}{2}\begin{cases} 1 & m=n, \\ 0 & m\neq n, \end{cases} \tag{26}$$

(25) produces the formula

$$a_n = \frac{2}{l}\int_0^l u_0(x)\sin\frac{n\pi x}{l}\, dx. \tag{27}$$

The condition (25) says that the **eigenfunctions** $X_n(x) = \sin(n\pi x/l)$ and $X_m(x) = \sin(m\pi x/l)$ with $n \neq m$ are **orthogonal** for the **scalar product**:

$$(f,g) = \int_0^l f(x)g(x)\, dx. \tag{28}$$

Putting together (24) and (27), we find

$$u(x,t) = \sum_{n=1}^{\infty}\left(\frac{2}{l}\int_0^l u_0(s)\sin\frac{n\pi s}{l} ds\right) e^{-n^2\pi^2 kt/l^2}\sin\frac{n\pi x}{l}. \tag{29}$$

There are several questions that we should be able to answer before we become satisfied with the solution (29):

1. For which functions $u_0(x)$ does the ***Fourier sine series*** (25) with coefficients (27) converge? What do we mean by convergence?

2. Is the Fourier sine series (29) a differentiable function that solves the IBVP (14) with $f = 0$?

We will deal with these questions later. Here it suffices to say that, provided $u_0(x) = f(x)$ is ***piecewise smooth*** ($f(x)$ and $f'(x)$ are both continuous in $(0,l)$ except in finitely many points ξ where they have finite jump discontinuities, $[f(\xi)] \equiv \lim_{\epsilon\to 0+}[f(\xi+\epsilon) - f(\xi-\epsilon)] \neq 0$), the Fourier sine series converges to $f(x)$ in all points where $f(x)$ is continuous, and it converges to the average value $[f(x+) + f(x-)]/2$ in points where $f(x)$ has a jump discontinuity.

This notion of ***pointwise convergence*** will be sufficient for our purposes in this course. Be warned that there are other important notions of convergence that may be quite useful in certain cases.

3. Homogeneous heat equation with Neumann boundary conditions

If the boundary conditions are (15) (**Neumann**) instead of Dirichlet, a repetition of the procedure followed to derive the eigenfunctions (22), yields the following eigenvalue-eigenfunction pairs [2];

$$\lambda_n = \frac{n^2\pi^2}{l^2}, \quad X_n(x) = \cos\frac{n\pi x}{l}, \quad n = 0, 1, \dots, \tag{30}$$

instead of (22).

This leads to the **Fourier cosine series** solution

$$u(x,t) = \frac{1}{l}\int_0^l u_0(s)ds + \sum_{n=1}^{\infty}\left(\frac{2}{l}\int_0^l u_0(s)\cos\frac{n\pi s}{l}ds\right)e^{-n^2\pi^2 kt/l^2}\cos\frac{n\pi x}{l}. \tag{31}$$

Unlike in the case of Dirichlet boundary conditions, the temperature converges to the average of the initial temperature profile and not to zero temperature: **a thermally insulated rod remembers some features of its initial temperature even after infinite time**.

4. Homogeneous heat equation with periodic boundary conditions

Let us assume that we have a thin rod that is curved and closed as a ring with large radius. The ring comprises the interval $-l < x < l$ and we have to solve the homogeneous heat equation with **periodic boundary conditions**:

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2}, \quad \begin{cases} u(-l,t) = u(l,t), \\ \frac{\partial u}{\partial x}(-l,t) = \frac{\partial u}{\partial x}(l,t). \end{cases} \tag{32}$$

Now the eigenvalue problem is (20) with periodic boundary conditions as in (32). Inserting the general solution of (20),

$$X(x) = c_1\cos(\sqrt{\lambda}x) + c_2\sin(\sqrt{\lambda}x),$$

in the periodic boundary conditions, we obtain

$$2c_2\sin(l\sqrt{\lambda}) = 0, \quad 2c_1\sqrt{\lambda}\sin(l\sqrt{\lambda}) = 0,$$

which produce the following eigenvalues and eigenfunctions:

$$\lambda_n = \frac{n^2\pi^2}{l^2}, \quad X_n^{(1)}(x) = \cos\frac{n\pi x}{l}, \quad X_n^{(2)}(x) = \sin\frac{n\pi x}{l}, \quad n = 0, 1, \dots. \tag{33}$$

Note that the eigenvalue $\lambda_0 = 0$ has a single eigenfunction $X_0 = 1$, whereas all the other eigenvalues have two independent eigenfunctions associated to them, thereby having multiplicity two.

According to the superposition principle, **the general solution of the homogeneous heat equation** is now

$$u(x,t) = a_0 + \sum_{n=1}^{\infty} a_n \cos\frac{n\pi x}{l} e^{-n^2\pi^2 kt/l^2} + \sum_{n=1}^{\infty} b_n \sin\frac{n\pi x}{l} e^{-n^2\pi^2 kt/l^2}. \tag{34}$$

Using the **orthogonality of the eigenfunctions**

$$\int_{-l}^{l} \cos\frac{n\pi x}{l} \cos\frac{m\pi x}{l} dx = \begin{cases} 0 & n \neq m \\ l & n = m \neq 0 \\ 2l & n = m = 0 \end{cases} \tag{35}$$

$$\int_{-l}^{l} \sin\frac{n\pi x}{l} \sin\frac{m\pi x}{l} dx = \begin{cases} 0 & n \neq m \\ l & n = m \neq 0 \end{cases} \tag{36}$$

$$\int_{-l}^{l} \cos\frac{n\pi x}{l} \sin\frac{m\pi x}{l} dx = 0, \tag{37}$$

in the initial condition, we find the **Fourier coefficients**

$$\begin{aligned} a_0 &= \frac{1}{2l}\int_{-l}^{l} u_0(x)dx, \\ a_n &= \frac{1}{l}\int_{-l}^{l} u_0(x)\cos\frac{n\pi x}{l}dx, \\ b_n &= \frac{1}{l}\int_{-l}^{l} u_0(x)\sin\frac{n\pi x}{l}dx. \end{aligned} \tag{38}$$

Equations (34) and (38) become

$$\begin{aligned} u(x,t) &= \frac{1}{2l}\int_{-l}^{l} u_0(s)ds + \sum_{n=1}^{\infty}\Bigg\{e^{-n^2\pi^2 kt/l^2}\left[\left(\frac{1}{l}\int_{-l}^{l} u_0(s)\sin\frac{n\pi s}{l}\,ds\right)\sin\frac{n\pi x}{l}\right. \\ &+ \left.\left(\frac{1}{l}\int_{-l}^{l} u_0(s)\cos\frac{n\pi s}{l}\,ds\right)\cos\frac{n\pi x}{l}\right]\Bigg\} \\ &= \int_{-l}^{l}\left\{\frac{1}{2l} + \frac{1}{l}\sum_{n=1}^{\infty} e^{-n^2\pi^2 kt/l^2}\cos\frac{n\pi(x-s)}{l}\right\} u_0(s)\,ds. \end{aligned} \tag{39}$$

As $t \to \infty$, $u(x,t) \to (2l)^{-1}\int_{-l}^{l} u_0(s)ds$, which is the equilibrium temperature for the circular rod: it is an average of the initial temperature distribution.

5. *Inhomogeneous problems*

Let us consider the inhomogeneous IBVP

$$\begin{aligned} \frac{\partial u}{\partial t} - k\frac{\partial^2 u}{\partial x^2} &= f(x,t), \quad 0 < x < l, \quad t > t_0, && (40) \\ u(x,t_0) &= u_0(x), \quad 0 < x < l, && (41) \\ u(0,t) &= T_0(t), \quad t > t_0, && (42) \\ u(l,t) &= T_1(t), \quad t > t_0 && (43) \end{aligned}$$

Here **we cannot separate variables**. However, we can **expand the solution in a Fourier sine series** (appropriate for Dirichlet boundary conditions) as:

$$u(x,t) = \sum_{n=1}^{\infty} b_n(t) \sin\frac{n\pi x}{l}, \tag{44}$$

where now we do not know its time dependence.

Note that the orthogonality of the sine functions give the formula

$$b_n(t) = \frac{2}{l}\int_0^l u(x,t)\sin\frac{n\pi x}{l}\,dx, \tag{45}$$

for the Fourier coefficients of the solution.

We now multiply (40) by $(2/l)\sin(n\pi x/l)$ and integrate the result from 0 to l, thereby obtaining

$$\begin{aligned} \frac{db_n}{dt} - \frac{2k}{l}\sin\frac{n\pi x}{l}\,\frac{\partial u}{\partial x}(x,t)\Big|_0^l + \frac{2n\pi k}{l^2}\cos\frac{n\pi x}{l}u(x,t)\Big|_0^l + \frac{2kn^2\pi^2}{l^3}\int_0^l u(x,t)\sin\frac{n\pi x}{l}dx \\ = \frac{2}{l}\int_0^l f(x,t)\sin\frac{n\pi x}{l}dx, \end{aligned}$$

after integrating twice by parts.

Using the boundary conditions (42) and (43) and the formula (45) in this equation, we find the ODE:

$$\frac{db_n}{dt} + \frac{n^2\pi^2 k}{l^2}b_n = \frac{2kn\pi}{l^2}[T_0(t) - (-1)^n T_1(t)] + f_n(t), \quad f_n(t) = \frac{2}{l}\int_0^l f(x,t)\sin\frac{n\pi x}{l}\,dx. \tag{46}$$

This is a **first-order linear ODE** to be solved with the initial condition

$$b_n(0) = \frac{2}{l}\int_0^l u_0(x,)\sin\frac{n\pi x}{l}\,dx. \tag{47}$$

The solution of this IVP is

$$b_n(t) = b_n(0)e^{-n^2\pi^2 kt/l^2} + \int_0^t \left\{\frac{2kn\pi}{l^2}[T_0(s) - (-1)^n T_1(s)] + f_n(s)\right\} e^{-n^2\pi^2 k(t-s)/l^2}ds. \tag{48}$$

Equations (44) and (48) are the solution of the IBVP (40)-(43) [2].

B. Properties of Fourier series

Consider the Fourier series associated to a function $f(x)$ on the interval $(-1, 1)$:

$$f(x) \sim a_0 + \sum_{n=1}^{\infty}[a_n \cos(n\pi x) + b_n \sin(n\pi x)], \tag{49}$$

where the coefficients are given by the usual formulas:

$$\begin{aligned} a_0 &= \frac{1}{2}\int_{-1}^{1} f(x)dx, \\ a_n &= \int_{-1}^{1} f(x)\cos(n\pi x)dx, \\ b_n &= \int_{-1}^{1} f(x)\sin(n\pi x)dx. \end{aligned} \tag{50}$$

In (48), $\sim$ means that $f(x)$ is on the left hand side and the Fourier series of $f(x)$ (on the interval $-1 \leq x \leq 1$) is on the right hand side (even if the series diverges) but the two functions may be completely different. The **symbol** $\sim$ is read as "**has the Fourier series (on a given interval)**".

1. *Fourier series in dimensional units*

In dimensional units, the function $f(x)$ is defined on an interval $(-l, l)$.
Replacing x/l instead of x in (49) and (50), we obtain

$$f(x) \sim a_0 + \sum_{n=1}^{\infty}\left[a_n \cos\left(\frac{n\pi x}{l}\right) + b_n \sin\left(\frac{n\pi x}{l}\right)\right], \tag{51}$$

with coefficients given by:

$$\begin{aligned} a_0 &= \frac{1}{2l}\int_{-l}^{l} f(x)dx, \\ a_n &= \frac{1}{l}\int_{-l}^{l} f(x)\cos\left(\frac{n\pi x}{l}\right)dx, \\ b_n &= \frac{1}{l}\int_{-l}^{l} f(x)\sin\left(\frac{n\pi x}{l}\right)dx. \end{aligned} \tag{52}$$

2. *Pointwise convergence theorem*

If $f(x)$ is piecewise smooth on the interval $-l \leq x \leq l$, then the Fourier series of $f(x)$ converges

1. to the **periodic extension** of $f(x)$, where the periodic extension is continuous;

2. to the average of the two limits,

$$\frac{f(x+) + f(x-)}{2},$$

   where the periodic extension has a jump discontinuity.

Here a **piecewise smooth** $f(x)$ **means** that f and df/dx are both piecewise continuous, i.e.:
(i) they are continuous at all but a finite number of points in $(-l, l)$;
(ii) every discontinuity in $(-l, l)$ is a jump discontinuity;
(iii) their limits as $x \to -l+$ and as $x \to l-$ exist.
For a proof of the pointwise convergence theorem see chapter 9 of [1].
The following results are a direct consequence of the Fourier pointwise convergence theorem:

a) If $f : (-l, l) \to \mathbb{R}$ is continuous and piecewise smooth, then its periodic extension is continuous everywhere except (possibly) at the points $\pm l, \pm 3l, \ldots$.
   It follows that the Fourier series of f converges to $f(x)$ for all $-l < x < l$.

b) If $f : [-l, l] \to \mathbb{R}$ is continuous and piecewise smooth, and $f(-l) = f(l)$, then its periodic extension is continuous everywhere, and therefore the Fourier series of f converges to $f(x)$ for all $-l \leq x \leq l$.

c) If $f : [0, l] \to \mathbb{R}$ is continuous and piecewise smooth, then f_{odd}, the periodic extension of its odd extension, is continuous everywhere except (possibly) at the points $0, \pm l, \pm 2l, \ldots$.
   As a consequence, the Fourier sine series of f converges to $f(x)$ for all $0 < x < l$.

d) If $f : [0, l] \to \mathbb{R}$ is continuous and piecewise smooth, and $f(0) = f(l) = 0$, then f_{odd} is continuous everywhere. Then the Fourier sine series of f converges to $f(x)$ for all $0 \leq x \leq l$.

e) If $f : [0, l] \to \mathbb{R}$ is continuous and piecewise smooth, then f_{even}, the periodic extension of its even extension, is continuous everywhere. Then the Fourier cosine series of f converges to $f(x)$ for all $0 \leq x \leq l$.

It can be proved that when the periodic extensions of a piecewise smooth $f(x)$, or of its even or odd extensions, are continuous, the corresponding Fourier series converge uniformly to f, [1]. Then the Fourier series can be differentiated term by term and the resulting series converges to $f'(x)$ whenever the derivative is continuous.

3. ***Sketching Fourier series***

We can sketch Fourier series by drawing the corresponding periodic extensions and marking with a cross the points at which the series converges at discontinuity points of the periodic extension of $f(x)$.

4. ***Term-by-term differentiation of Fourier series***

If the periodic extension of a continuous function has a Fourier series with jump discontinuities at the ends of the interval $(-l, l)$, then it cannot be differentiated term by term.
To see why, take the Fourier series of $f'(x)$:

$$f'(x) \sim A_0 + \sum_{n=1}^{\infty} \Big[A_n \cos\Big(\frac{n\pi x}{l}\Big) + B_n \sin\Big(\frac{n\pi x}{l}\Big)\Big]. \tag{53}$$

The Fourier coefficients can be calculated by integration by parts using (52) to simplify the result:

$$\begin{aligned} A_0 &= \frac{1}{2l}\int_{-l}^{l} f'(x)dx = \frac{f(l)-f(-l)}{2l}, \\ A_n &= \frac{1}{l}\int_{-l}^{l} f'(x)\cos\Big(\frac{n\pi x}{l}\Big)dx = \frac{f(l)-f(-l)}{l}\cos(n\pi) + n\pi b_n, \\ B_n &= \frac{1}{l}\int_{-l}^{l} f'(x)\sin\Big(\frac{n\pi x}{l}\Big)dx = -n\pi a_n. \end{aligned} \tag{54}$$

Clearly we need $f(-l) = f(l)$ for term-by-term differentiation to hold.

5. ***Term-by-term integration of Fourier series***

We can integrate term by term the Fourier series of a piecewise smooth function $f(x)$ and the result is a convergent series that always converges to the integral of $f(x)$ for $-l \leq x \leq l$

even if the original Fourier series has jump discontinuities. The new series formed by term-by-term integration is continuous, but it may not be a Fourier series.
See a proof of this statement in section 3.5 of [2].

III. SUPPLEMENTARY MATERIAL: FINITE DIFFERENCE SOLUTION OF THE HEAT EQUATION

We want to find the numerical solution of the following Dirichlet problem in dimensional units

$$\begin{aligned} \frac{\partial u}{\partial t} &= k\frac{\partial^2 u}{\partial x^2}, \quad 0 < x < l, \quad t > 0, \\ u(x,t_0) &= f(x), \quad 0 < x < l, \\ u(0,t) &= 0, \quad t > 0, \\ u(l,t) &= 0, \quad t > 0. \end{aligned} \tag{55}$$

This problem is quite simple and it is indifferent to rewrite it in dimensional units. Please keep in mind that nondimensionalizing before solving numerically is a good idea [2].

A. Explicit scheme

The simplest numerical scheme consists of using **forward differences** in time and **centered differences** in space:

$$\frac{\partial u}{\partial t}(x_j,t_j) = \frac{u(x_j,t_j+\Delta t)-u(x_j,t_j)}{\Delta t} - \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2}(x_j,\tilde{t}_j), \tag{56}$$

$$\frac{\partial^2 u}{\partial x^2}(x_j,t_j) = \frac{u(x_j+\Delta x,t_j)+u(x_j-\Delta x,t_j)-2u(x_j,t_j)}{(\Delta x)^2} - \frac{(\Delta x)^2}{12}\frac{\partial^4 u}{\partial x^4}(\tilde{x}_j,t_j), \tag{57}$$

where $t_j < \tilde{t}_j < t_j + \Delta t$, $x_j < \tilde{x}_j < x_j + \Delta x$, and we have discretized time and space according to
$0 = t_0 < t_1 = t_0 + \Delta t < \ldots < t_M = t_0 + M\Delta t = T$, and
$0 = x_0 < x_1 = x_0 + \Delta x < \ldots < x_N = x_0 + N\Delta x = l$.
We now substitute (56) and (57) into (55), drop the error terms and use the notation

$$u(x_j,t_m) = U_j^m \tag{58}$$

(indicating the temperature at the mesh point x_j at time t_m), in the result.

We obtain the following difference scheme:

$$U_j^{m+1} = U_j^m + r\,(U_{j+1}^m + U_{j-1}^m - 2U_j^m), \tag{59}$$

$$U_j^0 = f(x_j) \equiv f_j\,(j = 1, \ldots, N-1), \tag{60}$$

$$U_0^m = 0, \quad U_N^m = 0\,(m = 1, \ldots, M-1), \tag{61}$$

in which r in the **dimensionless parameter**

$$r = k\frac{\Delta t}{(\Delta x)^2}. \tag{62}$$

The scheme (59) marches forward in time starting from the initial condition (60) and taking into account the Dirichlet boundary conditions (61) at $j = 0$ and $j = N$.

To calculate the temperature at (x_j, t_{m+1}) we need the temperature at (x_j, t_m) and at the adjacent nodes (x_{j-1}, t_m) and (x_{j+1}, t_m).

Clearly the **domain of influence of a point** (x_j, t_m) is a triangular region whose borders expand at a **numerical velocity**

$$\frac{\Delta x}{\Delta t} = \frac{k\Delta x}{r(\Delta x)^2} = \frac{k}{r\,\Delta x}. \tag{63}$$

As $\Delta x \to 0$, with fixed r, the **numerical velocity** approaches infinity which agrees with the fact that the heat equation propagates disturbances with infinite velocity.

B. Stability analysis

The discrete scheme (59) can be solved by **separation of variables**

$$U_j^m = e^{i\alpha x} R^{t/\Delta t} = e^{i\alpha j\Delta x} R^m. \tag{64}$$

Inserting (64) into (59) and canceling $e^{i\alpha x}R^m$, we get

$$R = 1 + r(e^{i\alpha\Delta x} + e^{-i\alpha\Delta x} - 2) = 1 - 2r[1 - \cos(\alpha\Delta x)] = 1 - 4r\sin^2\left(\frac{\alpha\Delta x}{2}\right). \tag{65}$$

We have used Euler's formula: $e^{\pm i\omega} = \cos(\omega) \pm i\sin(\omega)$, with $\omega \in \mathbb{R}$.

R is the same for positive or negative α. Thus a linear combination of $e^{\pm i\alpha x}$ can be used as a solution. The boundary condition $U_0^m = 0$ implies that $\sin(\alpha x)$ is an appropriate solution while $U_N^m = 0$ implies $\alpha = n\pi/l = n\pi/(N\Delta x)$, $n = 1, \ldots, N-1$.

Then we find

$$U_j^m = \sin\frac{n\pi x}{l}\,R^m = \sin\frac{n\pi j}{N}\,R^m, \tag{66}$$

where R is given by (65), then:

$$R_n = 1 - 2r\left[1 - \cos\left(\frac{n\pi\Delta x}{l}\right)\right] = 1 - 4r\sin^2\left(\frac{n\pi}{2N}\right), \tag{67}$$

with $n = 1, \ldots, N-1$ and $n\Delta x = l$.

The **general solution** is found by the **superposition principle**:

$$U_j^{(m)} = \sum_{n=1}^{N-1} \beta_n \sin\frac{n\pi x}{l} R_n^m, \quad R_n^m = \left[1 - 4r\sin^2\left(\frac{n\pi}{2N}\right)\right]^{t/\Delta t} \quad r = \frac{k\Delta t}{(\Delta x)^2}. \tag{68}$$

The coefficients β_n are determined from the initial condition using the orthogonality of the eigenfunctions.

On the other hand, if $|R| < 1$, the solution of the discrete scheme tends to zero as $t \to \infty$ and we say that the numerical scheme is ***stable***. Otherwise the scheme is ***unstable***.

Clearly (67) implies that $R_n \le 1$, so we only have to check that $R_n \ge -1$:

$$r \le \frac{1}{2\sin^2\frac{n\pi}{2N}}, \quad n = 1, \ldots, N-1. \tag{69}$$

This condition is satisfied for all n provided

$$r \le \frac{1}{2} < \frac{1}{2\sin^2\frac{(N-1)\pi}{2N}}. \tag{70}$$

For large N, we get $r \le 1/2$ anyway.

If $r > 1/2$, then some R_n may become smaller than -1 and the numerical solution will contain a divergent oscillation, which is a ***numerical instability***, and does not reflect the behavior of the solution of the heat equation.

The numerical instability is characterized by an oscillation which is divergent in time, $R < -1$, and is rapidly oscillatory ($n = N-1$) in space.

The restriction $r \le 1/2$ becomes

$$\Delta t \le \frac{(\Delta x)^2}{2k}, \tag{71}$$

which is a practical constraint on numerical computations: **the time steps cannot become too large for otherwise the scheme becomes unstable**.

If Δx is sufficiently small, (71) implies a much smaller time step and the **explicit finite difference scheme** (59) is quite expensive.

To minimize calculation time, it is a good idea to use $r = 1/2$, so that (59) becomes

$$U_j^{m+1} = \frac{U_{j+1}^m + U_{j-1}^m}{2}, \tag{72}$$

and the temperature at time $(m+1)\Delta t$ is the average of the temperatures to the left and right at the previous time $m\Delta t$.

Remark: Simplified stability analysis.

If we do not impose the boundary conditions, $R \geq -1$ with R given by (65), yields

$$r \leq \frac{1}{2\sin^2(\alpha\Delta x/2)},$$

and the condition $r \leq 1/2$ is again obtained.

[1] M. S. Gockenbach, Partial differential equations. SIAM, 2002. Chapters 6 and 9.

[2] R. Haberman, Elementary applied partial differential equations. 3rd ed. Prentice Hall, 1998. Chapters 2, 3 and 8.