VIII.

II. Heat Equation via Fourier Series [cont.]

III. Heat Equation via FT

IV. Schrödinger Equation

We Find the differential equation for $b_n(t)$ from the original partial differential equation:

$$\partial_t u = \partial^2_{xx} u + F$$

We study the derivatives of u as Fourier series

$$\partial_t u(x,t) = \sum_{n=1}^{\infty} b_n'(t) \sin\left(\frac{\pi n}{L} x\right)$$

$$\partial_x u(x,t) = \sum_{n=1}^{\infty} b_n(t) \frac{\pi n}{L} \cos\left(\frac{\pi n}{L} x\right)$$

$$\partial^2_{xx} u(x,t) = \sum_{n=1}^{\infty} b_n(t) \frac{-\pi^2 n^2}{L^2} \sin\left(\frac{\pi n}{L} x\right)$$

We write the heat equation in terms of Fourier sine series:

$$\sum_{n=1}^{\infty} b_n'(t) \sin\left(\frac{\pi n}{L} x\right) = \sum_{n=1}^{\infty} b_n(t) \frac{-\pi^2 n^2}{L^2} \sin\left(\frac{\pi n}{L} x\right) + \sum_{n=1}^{\infty} \beta_n(t) \sin\left(\frac{\pi n}{L} x\right)$$

We have two Fourier sine series on both sides, the corresponding coefficients must be the same for each n:

$$b_n'(t) = -b_n(t) \cdot \frac{\pi^2 n^2}{L^2} + \beta_n(t)$$

← Differential Equation for $b_n(t)$

Using the initial data:

$$\sum_{n=1}^{\infty} b_n(0) \sin\left(\frac{\pi n}{L} x\right) = \sum_{n=1}^{\infty} b_n^0 \sin\left(\frac{\pi n}{L} x\right)$$

Hence

$$b_n(0) = b_n^0$$

← initial value at $t = 0$

We have decoupled the problem into independent Cauchy problems, one for each frequency.

$$b_n'(t) = -\left(\frac{\pi n}{L}\right)^2 b_n(t) + \beta_n(t), \qquad b_n(0) = b_n^0$$

These first-order initial value problems are solved by:

$$b_n(t) = b_n^0 \, e^{-\left(\frac{\pi n}{L}\right)^2 t} + \int_0^t \beta_n(s) \, e^{-\left(\frac{\pi n}{L}\right)^2 (t-s)} \, ds$$

[see discussion of first-order initial value problems]

3. Having found the Fourier coefficients, we assemble the solution of the heat equation:

$$u(x,t) = \sum_{n=1}^{\infty} b_n(t) \sin\left(\frac{\pi n}{L} x\right) \qquad \begin{array}{l} 0 \leq x \leq L \\ t \geq 0 \end{array}$$

$$= \sum_{n=1}^{\infty} \left(b_n^0 e^{-\left(\frac{\pi n}{L}\right)^2 t} + \int_0^t \beta_n(s) e^{-\left(\frac{\pi n}{L}\right)^2 (t-s)} ds \right) \sin\left(\frac{\pi n}{L} x\right)$$

- This solves the heat equation + B.C. + initial values
- This exemplifies a "separation of variables": we write the solution as a sum of products

$$u(x,t) = \sum_{n=1}^{\infty} \underbrace{b_n(t)}_{\text{depends only on } t} \underbrace{\sin\left(\frac{\pi n}{L} x\right)}_{\text{depends only on } x}$$

- We have decomposed the heat equation into simpler subproblems, one for each frequency.

- Comparison with Poisson problem:
  - decompose solution / data / equation into Fourier series
  - Poisson problem: find coefficients by linear equation
  - Heat problem: " " by solving ordinary diff'eq.

Similarly, one can solve:

Wave equation: $\partial_{tt}^2 u = \partial_{xx}^2 u + f$

Biharmonic diffusion: $\partial_t u = \partial_{xxxx}^4 u + f$

Schrödinger Equation: $i \partial_t u = \partial_{xx}^2 u$

VIII. 3. Heat Equation over $\mathbb{R}$ using Fourier transformations

Having addressed the heat equation over intervals, how do we address the heat equation over $\mathbb{R}$?

Let $f : \mathbb{R} \to \mathbb{R}$ be a source term, and let $k \geq 0$ be a material coefficient. We want to solve

$$\partial_t u(x,t) = k^2 \partial_{xx} u(x,t) + f(x,t) \qquad \begin{array}{c} -\infty < x < \infty \\ t > 0 \end{array}$$

with initial conditions at time $t=0$

$$u(x,0) = u_0(x) \qquad -\infty < x < \infty$$

Here, no boundary data because there is no boundary. However, the solution that we find will satisfy a decay condition towards $\pm\infty$.

Apply the Fourier transform (FT) in x:

$$\partial_t \hat{u}(\alpha, t) = k^2 (i\alpha)^2 \hat{u}(\alpha, t) + \hat{f}(\alpha, t)$$

FT in x, can be switched with ∂_t

FT in x, turns ∂_{xx} into $(i\alpha)^2$

FT in x

Initial values after Fourier transform:

$$\hat{u}(\alpha, 0) = \hat{u}_0(\alpha)$$

Heat equation over $\mathbb{R}$ from "frequency perspective"

NB: No x derivatives, only time derivatives

For each frequency $\alpha \in \mathbb{R}$, we have an independent Cauchy problem.

For each $\alpha \in \mathbb{R}$, we solve

$$\partial_t \hat{u}(\alpha, t) = -k^2 \alpha^2 \hat{u}(\alpha, t) + \hat{f}(\alpha, t), \qquad t > 0$$

$$\hat{u}(\alpha, 0) = \hat{u}_0(\alpha)$$

For each fixed $\alpha \in \mathbb{R}$, we solve the Cauchy problem

$$\hat{u}(\alpha, t) = \hat{u}_0(\alpha)\, e^{-k^2\alpha^2 t} + \int_0^t \hat{f}(\alpha, s)\, e^{-k^2\alpha^2(t-s)}\, ds$$

[see discussion of first-order initial value problems]

Having found a formula for $\hat{u}(\alpha, t)$ for all $\alpha \in \mathbb{R}$ and $t \geq 0$, we apply the inverse FT in α to get back to $u(x, t)$.

$$u(x,t) = \mathcal{F}^{-1}\left[u(\alpha,t) \right]$$

$$= \mathcal{F}^{-1}\left[\underbrace{\hat{u}_0(\alpha)}_{\mathcal{F}[u_0]} \, \underbrace{e^{-k^2\alpha^2 t}}_{\mathcal{F}[?]} \right] + \mathcal{F}^{-1}\left[\int_0^t \underbrace{\hat{f}(\alpha,s)}_{\mathcal{F}[f]} \, \underbrace{e^{-k^2\alpha^2(t-s)}}_{\mathcal{F}[?]} \, ds \right]$$

We notice that we can switch FT^{-1} in α with time integral

$$\mathcal{F}^{-1} \int_0^t \cdots = \int_0^t \mathcal{F}^{-1} \cdots$$

We know (FT table) or compute explicitly

$$e^{-\omega^2 x^2} \xrightarrow{FT} \frac{1}{\sqrt{2}\,|\omega|} e^{-\alpha^2/4\omega^2}$$

We use that to see:

$$\frac{e^{-\frac{x^2}{4k^2t}}}{\sqrt{2k^2t}} \overset{FT}{\rightsquigarrow} e^{-\alpha^2k^2t} \qquad \omega^2 = \frac{1}{4k^2t}$$

Recall the convolution formula

$$\mathcal{F}[f] \cdot \mathcal{F}[g] = \frac{1}{\sqrt{2\pi}} \mathcal{F}[f * g]$$

With that, we compute

$$u(x,t) = u_0(x) * \frac{e^{-\frac{x^2}{4k^2t}}}{\sqrt{4\pi k^2 t}} + \int_0^t f(x,s) * \frac{e^{-\frac{x^2}{4k^2(t-s)}}}{\sqrt{4\pi k^2 (t-s)}} \, ds$$

$$= \int_{-\infty}^{+\infty} u_0(y) \frac{e^{-\frac{(x-y)^2}{4k^2t}}}{\sqrt{4\pi k^2 t}} \, dy + \int_0^t \int_{-\infty}^{+\infty} f(y,s) \frac{e^{-\frac{(x-y)^2}{4k^2(t-s)}}}{\sqrt{4\pi k^2 (t-s)}} \, dy \, ds$$

Remarks: • The "heat kernel" is the function

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

The heat kernel appears in the solution theory of many PDE.

- The solution formula for the H.E. might be tedious to use explicitly but can be evaluated approximately using <u>numerical integration</u> on a computer.

VIII. 4. Schrödinger Equation

We study the Schrödinger equation over an interval $[0, L]$ with a linear potential term:

$$i\, \partial_t u(x,t) = \partial_{xx}^2 u(x,t) - a u(x,t) + f(x,t).$$

potential term $a \geq 0$

We impose Dirichlet boundary conditions,

$$u(0,t) = 0, \qquad u(L,t) = 0, \qquad t > 0,$$

and initial values at $t = 0$:

$$u(x,0) = u_0(x), \qquad 0 \leq x \leq L.$$