Chapter 9 Partial Differential Equations

More than one independent variable. For $\varphi(x,y)$ $\frac{\partial \varphi}{\partial x}$ is the derivative of $\varphi(x,y)$ with respect to x while keeping y constant

PDE's :

- Laplace equation, $\nabla^2 \psi = 0$
  - electromagnetic phenomena; electrostatics, dielectrics, steady currents, magnetostatics
  - hydrodynamics
  - heat flow
  - gravitation
- Poisson's equation, $\nabla^2 \psi = -\frac{\rho}{\varepsilon_0}$
  - electrostatics with source term $-\rho/\varepsilon_0$
- Helmholtz and time-independent diffusion eq. $\nabla^2 \psi \pm k^2 \psi = 0$
  - elastic waves in solids (vibrating strings, bars, membranes)
  - acoustics (sound waves)
  - electromagnetic waves
  - nuclear reactors
- Time-dependent diffusion eq. $\nabla^2 \psi = \frac{1}{a^2} \frac{\partial \psi}{\partial t}$
- Time-dependent classical wave eq. $\frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} = \nabla^2 \psi$
- Klein-Gordon eq. $\partial^2 \psi = -\mu^2 \psi$
- Time-dependent Schrödinger eq. $-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = i\hbar \frac{\partial \psi}{\partial t}$

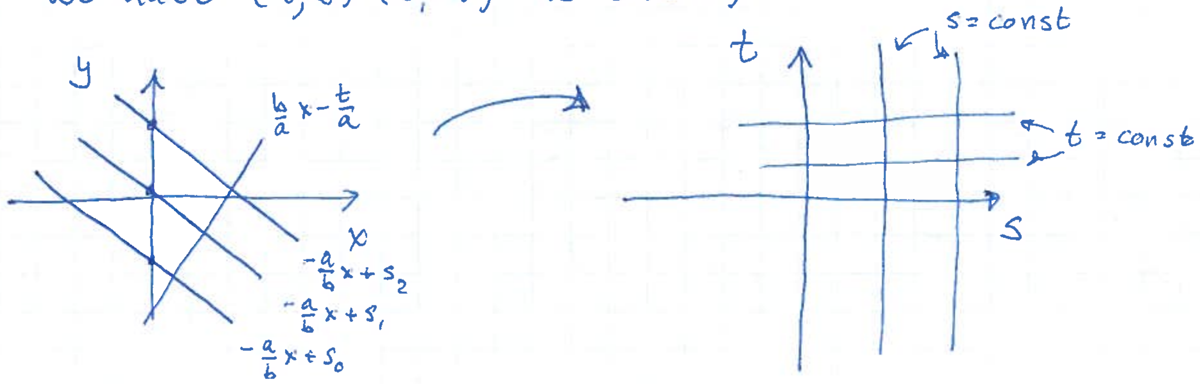
$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = E\psi \quad \text{(time-independent S.E)}$$

- Eq. for elastic waves, viscous fluids and telegraphy eq.
- Maxwell eq. for electric and magnetic fields
- Dirac equation for relativistic electron wave functions

First-order equations - Characteristics

The equation $\mathcal{L}\varphi = a\frac{\partial\varphi}{\partial x} + b\frac{\partial\varphi}{\partial y} = 0$ corresponds to a line along which a times the change with x is the negative of b times the change with y, or $(a,b)\left(\frac{\partial\varphi}{\partial x}, \frac{\partial\varphi}{\partial y}\right) = 0$. For a, b constant we have a straight line.

Change to a variable $s = ax+by$ along this line and take the orthogonal line $t = bx-ay$ as the other dimension (With $\hat{e}_x \cdot \hat{e}_y = 0$ we have $(a,b)\cdot(b,-a) = ab - ba = 0$)



Then $a\frac{\partial\varphi}{\partial x} + b\frac{\partial\varphi}{\partial y} = (a^2+b^2)\frac{\partial\hat{\varphi}}{\partial s}$

where $\hat{\varphi}(s,t) = \varphi(x(s,t), y(s,t)) = \varphi(x,y)$

and $$\left(\frac{\partial\varphi}{\partial x}\right)_y = \frac{\partial\varphi}{\partial s}\frac{\partial s}{\partial x} + \frac{\partial\varphi}{\partial t}\frac{\partial t}{\partial x} = a\left(\frac{\partial\varphi}{\partial s}\right)_t + b\left(\frac{\partial\varphi}{\partial t}\right)_s$$

$$\left(\frac{\partial\varphi}{\partial y}\right)_x = \frac{\partial\varphi}{\partial s}\frac{\partial s}{\partial y} + \frac{\partial\varphi}{\partial t}\frac{\partial t}{\partial y} = b\left(\frac{\partial\varphi}{\partial s}\right)_t - a\left(\frac{\partial\varphi}{\partial t}\right)_s$$

The equation $(a^2+b^2)\frac{\partial\hat{\varphi}}{\partial s} = 0$ is satisfied by <u>any</u> $f(t)$ so that $\hat{\varphi}(s,t) = f(t)$ and $\varphi(x,y) = f(bx-ay)$ for arbitrary function f

The curves of constant t are called <u>characteristic curves</u> or <u>characteristics</u> of the PDE and are the lines traced out by s with t constant.

Example 9.2.1

$$\mathcal{L}\varphi = a\frac{\partial \varphi}{\partial x} + b\frac{\partial \varphi}{\partial y} + q(x,y)\varphi = F(x,y)$$

$$\frac{\partial \varphi}{\partial x} + \frac{\partial \varphi}{\partial y} + (x+y)\varphi = 0$$

set $s = x+y$, $t = x-y$ $\Rightarrow$ $2\frac{\partial \varphi}{\partial s} + s\varphi = 0$

Separate $2\frac{d\varphi}{\varphi} + s\,ds = 0$ which integrates to

$$\ln\varphi = -\frac{s^2}{4} + C(t) \Rightarrow \varphi(s,t) = e^{-s^2/4} f(t)$$

$$s^2 = (x+y)^2 = x^2 + 2xy + y^2 = (x^2 - 2xy + y^2) + 4xy = t^2 + 4xy$$

$$\Rightarrow \varphi(x,y) = e^{-xy} f(x-y) \quad (f \text{ arbitrary})$$

Second-order equations

The equation $a^2\frac{\partial^2 \varphi(x,y)}{\partial x^2} - c^2\frac{\partial^2 \varphi(x,y)}{\partial y^2} = 0$ $(a, c$ real$)$

Since the derivatives commute we can write this as

hyperbolic $\left[a\frac{\partial}{\partial x} + c\frac{\partial}{\partial y}\right]\left[a\frac{\partial}{\partial x} - c\frac{\partial}{\partial y}\right]\varphi = 0$ and separate into two

equations
$$a\frac{\partial \varphi}{\partial x} + c\frac{\partial \varphi}{\partial y} = 0 \quad \text{and} \quad a\frac{\partial \varphi}{\partial x} - c\frac{\partial \varphi}{\partial y} = 0$$

with solutions $\varphi_1(x,y) = f(cx - ay)$ and $\varphi_2(x,y) = g(cx+ay)$
with f, g arbitrary functions. $ax+cy$ and $ax-cy$ are the characteristics.

The equation $a^2\frac{\partial^2 \varphi(x,y)}{\partial x^2} + c^2\frac{\partial^2 \varphi(x,y)}{\partial y^2} = 0$ $(a, c,$ real$)$

factorizes to $\left[a\frac{\partial}{\partial x} + ic\frac{\partial}{\partial y}\right]\left[a\frac{\partial}{\partial x} - ic\frac{\partial}{\partial y}\right]\varphi = 0$ elliptic

Equation of ellipse: $a^2x^2 + c^2y^2 = d$
— " — hyperbola: $a^2x^2 - c^2y^2 = d$

More general: $\mathcal{L} = a\frac{\partial^2 \varphi}{\partial x^2} + 2b\frac{\partial^2 \varphi}{\partial x \partial y} + c^2\frac{\partial^2 \varphi}{\partial y^2}$

This factorizes to

$$\alpha = \left(\frac{b+\sqrt{b^2-ac}}{\sqrt{c}}\frac{\partial}{\partial x} + \sqrt{c}\frac{\partial}{\partial y}\right)\left(\frac{b-\sqrt{b^2-ac}}{\sqrt{c}}\frac{\partial}{\partial x} + \sqrt{c}\frac{\partial}{\partial y}\right)$$

If $b^2 - ac > 0$ the coefficients are real $\rightarrow$ hyperbolic

$b^2 - ac < 0$ the coefficients form a complex conjugate pair $\rightarrow$ elliptic

$b^2 - ac = 0$ one linearly independent characteristic $\rightarrow$ parabolic

Elliptic Laplace $\nabla^2\psi = 0$, Poisson $\nabla^2\psi = -\rho/\varepsilon_0$

Hyperbolic Wave eq. $\nabla^2\psi = \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2}$

Parabolic Diffusion eq $a\frac{\partial\psi}{\partial t} = \nabla^2\psi$

Boundary conditions

Cauchy : The value of a function and normal derivative specified on the boundary (φ, $E_{\hat{n}}$)

Dirichlet : The value of a function specified on the boundary (potential φ)

Neumann : Normal derivative (normal gradient) specified on the boundary ($E_{\hat{n}}$)

Be careful when specifying boundary conditions. If the boundary curve (giving the initial conditions) is along a characteristic or intersects it more than once it ordinarily leads to inconsistencies.

See Table 9.1 for relations between PDE and boundary conditions

Separation of variables

Cartesian coordinates

Helmholtz equation $\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + k^2 \psi = 0$

There is no coupling of the different degrees of freedom

Make the Ansatz $\psi(x,y,z) = X(x)\,Y(y)\,Z(z)$

$$\Rightarrow YZ\frac{d^2X}{dx^2} + XZ\frac{d^2Y}{dy^2} + XY\frac{d^2Z}{dz^2} + k^2 XYZ = 0$$

divide by XYZ and ~~move~~ separate the ~~x~~ x-dependence

$$\frac{1}{X}\frac{d^2X}{dx^2} = -k^2 - \frac{1}{Y}\frac{d^2Y}{dy^2} - \frac{1}{Z}\frac{d^2Z}{dz^2} = -\ell^2$$ (has to be a constant since x, y, z vary freely)

$$\Rightarrow \frac{1}{X}\frac{d^2X}{dx^2} = -\ell^2$$

$$-k^2 - \frac{1}{Y}\frac{d^2Y}{dy^2} - \frac{1}{Z}\frac{d^2Z}{dz^2} = -\ell^2$$

Take the y-dependence $\frac{1}{Y}\frac{d^2Y}{dy^2} = -k^2 + \ell^2 - \frac{1}{Z}\frac{d^2Z}{dz^2} = -m^2$

$$\Rightarrow \frac{1}{Y}\frac{d^2Y}{dy^2} = -m^2 \quad ; \quad \frac{1}{Z}\frac{d^2Z}{dz^2} = -k^2 + \ell^2 + m^2 = -n^2$$

$$\Rightarrow \psi_{\ell m}(x,y,z) = X_\ell(x)\,Y_m(y)\,Z_n(z)$$

as long as boundary conditions are fulfilled and $k^2 = \ell^2 + m^2 + n^2$ then $\psi_{\ell m}$ solves the equation and since the equation is linear so does $\psi = \sum_{\ell,m} a_{\ell m}\psi_{\ell m}$ as the most general solution

Cylindrical coordinates

$$\nabla^2 \psi(\rho,\varphi,z) + k^2 \psi(\rho,\varphi,z) = 0 \qquad \text{Helmholtz equation}$$

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\varphi^2} + \frac{\partial^2\psi}{\partial z^2} + k^2\psi = 0$$

Again there is no mixing of degrees of freedom, no coupling

Ansatz: $\psi(\rho,\varphi,z) = P(\rho)\Phi(\varphi)Z(z)$

$$\Rightarrow \frac{\Phi Z}{\rho}\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right) + \frac{PZ}{\rho^2}\frac{d^2\Phi}{d\varphi^2} + P\Phi\frac{d^2Z}{dz^2} + k^2 P\Phi Z = 0$$

The z-dependence first: (divide by $P\Phi Z$)

$$k^2 + \frac{1}{\rho P}\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right) + \frac{1}{\rho^2\Phi}\frac{d^2\Phi}{d\varphi^2} = -\frac{1}{Z}\frac{d^2Z}{dz^2} = -l^2$$

$$\Rightarrow \frac{d^2Z}{dz^2} = l^2 Z$$

$$\frac{1}{\rho P}\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right) + \frac{1}{\rho^2\Phi}\frac{d^2\Phi}{d\varphi^2} + k^2 = -l^2$$

let $k^2 + l^2 = n^2$ and multiply by ρ^2

$$\frac{\rho}{P}\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right) + n^2\rho^2 = -\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2} = m^2$$

$$\Rightarrow \frac{d^2\Phi}{d\varphi^2} = -m^2\Phi$$

$$\rho\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right) + (n^2\rho^2 - m^2)P = 0 \qquad \text{Bessel's D.E.}$$

and $\psi_{mn}(\rho,\varphi,z) = P_{mn}(\rho)\Phi_m(\varphi)Z_n(z)$

General solution: $\psi = \sum_{m,n} a_{mn} P_{mn}(\rho)\Phi_m(\varphi)Z_n(z)$

Spherical polar coordinates

Helmholtz eq $\frac{1}{r^2\sin\vartheta}\left[\sin\vartheta\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial\psi}{\partial\vartheta}\right)+\right.$
$$\left.+\frac{1}{\sin\vartheta}\frac{\partial^2\psi}{\partial\varphi^2}\right]=-k^2\psi$$

Ansatz $\psi(r,\vartheta,\varphi)=R(r)\,\Theta(\vartheta)\,\Phi(\varphi)$

$$\Rightarrow \frac{1}{Rr^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{1}{\Theta r^2\sin\vartheta}\frac{d}{d\vartheta}\left(\sin\vartheta\frac{d\Theta}{d\vartheta}\right)+\frac{1}{\Phi r^2\sin^2\vartheta}\frac{d^2\Phi}{d\varphi^2}=-k^2$$

multiply by $r^2\sin^2\vartheta$ and separate the φ-dependence

$$\Rightarrow \frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2}=r^2\sin^2\vartheta\left[-k^2-\frac{1}{r^2R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{1}{r^2\sin^2\vartheta}\cdot\frac{1}{\Theta}\frac{d}{d\vartheta}\left(\sin\vartheta\frac{d\Theta}{d\vartheta}\right)\right]=$$
$$=-m^2$$

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2}=-m^2$$

divide the r,ϑ equation by $\sin^2\vartheta$ ~~and~~ and rearrange

$$-\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+k^2r^2=-\frac{1}{\sin\vartheta\,\Theta}\frac{d}{d\vartheta}\left(\sin\vartheta\frac{d\Theta}{d\vartheta}\right)+\frac{m^2}{\sin^2\vartheta}=Q$$

Associated Legendre eq. $\frac{1}{\sin\vartheta}\frac{d}{d\vartheta}\left(\sin\vartheta\frac{d\Theta}{d\vartheta}\right)-\frac{m^2}{\sin^2\vartheta}\Theta+Q\Theta=0$

with $Q=l(l+1)$

Radial equation: $\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+k^2R-\frac{QR}{r^2}=0$, spherical Bessel function if $k^2>0$

General solution

$$\psi(r,\vartheta,\varphi)=\sum_{Q,m}a_{Qm}R_Q(r)\,\Theta_{Qm}(\vartheta)\,\Phi_m(\varphi)$$

k^2 does not have to be a constant, for the hydrogen atom $k^2=f(r)$, i.e. the electrostatic potential

Since φ here is an angular variable we have a condition on m, since $\Phi(\varphi+2\pi)=\Phi(\varphi)$, i.e.

$$\frac{d^2\Phi}{d\varphi^2}=-m^2\Phi(\varphi)\Rightarrow\Phi(\varphi)=Ae^{\pm im\varphi}$$

Laplace and Poisson equations

Laplace $\nabla^2\varphi = 0$ has basic properties independent of coordinate system. Specifically, the second derivative is a measure of the curvature. In Cartesian coordinates

$$\nabla^2\varphi = 0 \longleftrightarrow \frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2} + \frac{\partial^2\varphi}{\partial z^2} = 0$$ shows that all

$\frac{\partial^2\varphi}{\partial x_i^2}$ cannot have the same sign. If one is positive at least one must be negative so that stationary points ($\frac{\partial\varphi}{\partial x_i} = 0 \quad i = x, y, z$) must be saddle points and not maxima or minima.

Laplace equation gives the static electric potential in charge-free regions $\longrightarrow$ the potential cannot have an extremum at a point where there is no charge & extrema of the electrostatic potential in a charge-free region must be on the boundary of the region.

Uniqueness of solutions of the Laplace and Poisson eq.

Assume Dirichlet boundary conditions for the entire closed boundary of the region. If φ_1 and φ_2 are distinct solutions to $\nabla^2\varphi = 0$ or $\nabla^2\varphi = -\rho/\varepsilon_0$ for the same boundary conditions then $\varphi = \varphi_1 - \varphi_2$ is a solution to $\nabla^2\varphi = 0$ with $\varphi = 0$ on the boundary. But φ cannot have extrema inside the region showing that $\varphi = 0$ everywhere and $\varphi_1 \equiv \varphi_2$

If instead we have Neumann boundary conditions on the entire closed boundary of its region then the difference of two solutions $\varphi = \varphi_1 - \varphi_2$ is also a solution but with zero Neumann boundary conditions.

Green's theorem relating a surface integral to integration over the enclosed volume:

$$\int_S u \nabla v \cdot d\underline{\sigma} = \int_V u \nabla^2 v \, d\tau + \int_V \nabla u \cdot \nabla v \, d\tau \qquad (3.86)$$

Take $u = v = \psi$

$$\underbrace{\int_S \psi \nabla \psi \cdot d\underline{\sigma}}_{(I)} = \underbrace{\int_V \psi \nabla^2 \psi \, d\tau}_{(II)} + \underbrace{\int_V \nabla \psi \cdot \nabla \psi \, d\tau}_{(III)}$$

(I) vanishes because of the zero Neumann condition ($\nabla_n \psi = 0$ on the boundary)

(II) vanishes because $\nabla^2 \psi = 0$

$\Rightarrow \int_V \nabla \psi \cdot \nabla \psi \, d\tau = \int_V \|\nabla \psi\|^2 d\tau = 0 \rightarrow \nabla \psi = 0$ everywhere inside

$\rightarrow \psi$ is constant

$\therefore$ The solution is unique apart for an additive constant to the potential.

Wave equation

1D: $\frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} = \frac{\partial^2 \psi}{\partial x^2}$

Hyperbolic eq. $\rightarrow$ Two characteristics which are the lines with constant $x - ct$ and $x + ct$ so the solution is

$$\psi(x,t) = f(x-ct) + g(x+ct) \quad \text{with } f, g \text{ arbitrary.}$$

$f(x-ct)$ represents a wave traveling forward ($+x$ direction) with constant velocity c, that is the whole function is shifted in x-position as t increases. $g(x+ct)$ travels in the negative x-direction. The sum $f(x-ct) + g(x+ct)$ will yield interference when the two waves occur in the same spatial region at the same time. If we have the same amplitude and sinusoidal waves we obtain standing waves:

$$\psi(x,t) = \sin(x-ct) + \sin(x+ct) = \sin x \cos ct - \cos x \sin ct + \sin x \cos ct + \cos x \sin ct = 2 \sin x \cos ct$$

Points where $\psi = 0$ (nodes) are now stationary while in a traveling wave they move with velocity $\pm c$

d'Alembert's Solution

We are given as initial value problem

(i) the entire spatial distribution $\psi(x,0)$ at time $t=0$ and

(ii) the time derivative of ψ at $t=0$ for the entire spatial distribution

We have the general solution $\psi(x,t) = f(x-ct) + g(x+ct)$

At $t=0$: $\psi(x,0) = f(x) + g(x)$ $\quad (*)$

$$\left.\frac{\partial \psi}{\partial t}\right|_{t=0} = -cf'(x) + cg'(x) \quad (**)$$

Integrate the derivative from $x-ct$ to $x+ct$ (ct is the distance the wave propagates in time t). Scale by $\frac{1}{2c}$ to combine with next step:

$$\frac{1}{2c}\int_{x-ct}^{x+ct} \frac{\partial \psi(x,0)}{\partial t}\,dx = \frac{1}{2}\int_{x-ct}^{x+ct}\{-f'(\xi) + g'(\xi)\}\,d\xi =$$

$$= \frac{1}{2}\{-f(x+ct) + f(x-ct) + g(x+ct) - g(x-ct)\} \quad (***)$$

From $(*)$ we have $\psi(x \pm ct, 0) = f(x \pm ct) + g(x \pm ct)$

x-coordinate

and $\frac{1}{2}[\psi(x+ct,0) + \psi(x-ct,0)] =$

$$= \frac{1}{2}\{f(x+ct) + g(x+ct) + f(x-ct) + g(x-ct)]$$

Add $(***)$ which gives for the RHS $f(x-ct) + g(x+ct) = \psi(x,t)$

so that

$$\psi(x,t) = \frac{1}{2}\{\psi(x+ct,0) + \psi(x-ct,0)\} + \frac{1}{2c}\int_{x-ct}^{x+ct}\frac{\partial \psi(x,0)}{\partial t}\,dx$$

Points at ct distance from x at time $t=0$

Integral over region of influence

Heat flow or Diffusion PDE

In homogeneous medium $\frac{\partial \psi}{\partial t} = a^2 \frac{\partial^2 \varphi}{\partial x^2} + b^2 \frac{\partial^2 \varphi}{\partial y^2} + c^2 \frac{\partial^2 \varphi}{\partial z^2}$

Rescale coordinates $x = a\xi$, $y = b\eta$, $z = c\zeta$ gives the equation for an isotropic medium (we have stretched the length scale differently in the different directions).

Specializing to 1-D: $\frac{\partial \psi}{\partial t} = a^2 \frac{\partial^2 \psi}{\partial x^2}$ where a measures the diffusivity or heat conductivity

Separate variables $\psi(x,t) = X(x)T(t) \Rightarrow XT' = a^2 X'' T$

so that $\frac{T'(t)}{T(t)} = a^2 \frac{X''(x)}{X(x)} = \beta$ (a constant)

We have (for $\beta \neq 0$) $T(t) = e^{\beta t}$ and $X(x) = e^{\pm \alpha x}$ with $\alpha^2 = \beta / a^2$

We need solutions that decay with time so $\beta < 0$. Set $\alpha = i\omega$ so that $\alpha^2 = -\omega^2$ (ω real)

This gives $\psi(x,t) = e^{i\omega x} e^{-\omega^2 a^2 t} = (\cos\omega x \pm i \sin\omega x) e^{-\omega^2 a^2 t}$

For $\beta = 0$ we obtain $T'(t) = 0$, $X''(x) = 0$ with solution

$\psi(x,t) = C_0' x + C_0$ which requires $C_0' = 0$ if the defining interva[l] is unbounded. C_0 will be the limiting value at long times.

A solution is given by $\psi(x,t) = (A\cos\omega x + B\sin\omega x) e^{-\omega^2 a^2 t} + C_0' x + C[_0]$

A, B, ω, C_0', C_0 are determined by the boundary conditions and initia[l] (or final) conditions. Take linear combinations:

Finite size problem: $\psi(x,t) = C_0 + \sum_n (A_n \cos\omega_n x + B_n \sin\omega_n x) e^{-\omega_n^2 a^2 t} + C_0[']$

Infinite length (ω continuous)

$$\psi(x,t) = C_0 + \int \{A(\omega)\cos\omega x + B(\omega)\sin\omega x\} e^{-\omega^2 a^2 t} d\omega$$

<u>Example</u>: $\psi_0(x,0) = 1$ for $|x| < 1$ and $\psi_0(x,0) = 0$ for $|x| \geq 1$

$\psi(\pm 1, t) = 0$. The initial temperature distribution is symmetric around $x = 0$ (even parity) so solutions must also be even.

We have the form of the solution

$$\psi(x,t) = (A\cos\omega x + B\sin\omega x)e^{-\omega^2 a^2 t} + C_0' x + C_0$$

The interval is infinite, so $C_0' = 0$

The solution will tend to $\psi(x, t\to\infty) = 0$ so $C_0 = 0$

The even functions on $[-1,1]$ having value 0 at $x = \pm 1$ are

$\cos\frac{l\pi x}{2}$ for l odd, so that at $t=0$ we have

$$\psi(x,0) = \sum_{l=0}^{\infty} a_l \cos\frac{(2l+1)\pi x}{2} \qquad -1 < x < +1$$

In this interval $\psi(x,0) = 1$. Find the coefficients a_l by projection $\left(\int_{-1}^{1} \cos\frac{(2p+1)\pi x}{2} \cdot \cos\frac{(2m+1)\pi x}{2}\, dx = \frac{1}{2}\int_{-1}^{1}\left\{ \cos(2p+2m+2)\frac{\pi x}{2} + \cos(2p-2m)\frac{\pi x}{2} \right\} dx = \begin{cases} 0, & p \neq m \\ 1, & p = m \end{cases} \right)$

$$a_l = \int_{-1}^{1} 1\cdot\cos\frac{\pi(2l+1)x}{2}\, dx = \frac{2}{(2l+1)\pi}\left[\sin\frac{\pi(2l+1)x}{2}\right]_{-1}^{1} = \frac{4}{(2l+1)\pi}\sin\frac{\pi(2l+1)}{2} = \frac{4(-1)^l}{(2l+1)\pi}$$

and we find $\psi(x,t) = \frac{4}{\pi}\sum_{l=0}^{\infty} \frac{(-1)^l}{2l+1}\cos\left[(2l+1)\frac{\pi x}{2}\right] e^{-t((2l+1)\pi a/2)^2}$

Alternative solutions

Seek solutions of functional form $\psi(x,t) = u(x/\sqrt{t}) \equiv u(\xi)$

set $\xi = \frac{x}{\sqrt{t}}$ (consider the dimensions $\frac{\partial^2\psi}{\partial x^2}$, $\frac{\partial\psi}{\partial t}$)

$$\left.\begin{aligned} \frac{\partial\psi}{\partial t} &= \frac{du}{d\xi}\frac{\partial\xi}{\partial t} = u'\left(-\frac{x}{2\sqrt{t^3}}\right) = -\frac{\xi}{2t}u' \\ \frac{\partial\psi}{\partial x} &= \frac{u'}{\sqrt{t}}, \quad \frac{\partial^2\psi}{\partial x^2} = \frac{u''}{t} \end{aligned}\right\} \Rightarrow \frac{a^2 u''}{t} = -\frac{\xi u'}{t}$$

So $2a^2 u''(\xi) + \xi u'(\xi) = 0$

separate $\frac{u''}{u'} = -\frac{\xi}{2a^2}$ and integrate $\Rightarrow \ln u'(\xi) = -\frac{\xi^2}{4a^2} + \ln C_1$

$u'(\xi) = C_1 \exp\left[-\frac{\xi^2}{4a^2}\right]$; Integrate again

$$u(\xi) = C_1 \int_0^{\xi} e^{-\xi^2/4a^2} d\xi + C_2$$

Initialize the solution to temperature $+1$ for $x>0$ and -1 for $x<0$ at time $t=0$ so $u(\infty)=1$ and $u(-\infty)=-1$

The integral $\int_0^{\infty} e^{-\xi^2/4a^2} d\xi$ $(\xi \to \infty)$ is obtained as

$$\left[\begin{array}{l} \frac{\xi}{2a} = q \\ d\xi = 2a\,dq \end{array}\right] \to 2a \int_0^{\infty} e^{-q^2} dq \equiv 2aI; \quad \text{Take } I^2 = \int_0^{\infty} e^{-q^2} dq \cdot \int_0^{\infty} e^{-p^2} dp =$$

$$= \int_0^{\infty}\int_0^{\infty} e^{-(q^2+p^2)} dq\,dp = \left[\begin{array}{c} q^2+p^2 = r^2 \\ dq\,dp = r\,dr\,d\varphi \\ \text{polar coord.} \end{array}\right] = \int_0^{\pi/2} d\varphi \int_0^{\infty} r e^{-r^2} dr =$$

$$= \frac{\pi}{2}\left[-\frac{1}{2} e^{-r^2}\right]_0^{\infty} = \frac{\pi}{4} \to I = \frac{\sqrt{\pi}}{2}$$

$$\therefore \int_0^{\infty} e^{-\xi^2/4a^2} d\xi = 2a \cdot \frac{\sqrt{\pi}}{2} = a\sqrt{\pi}$$

$$\text{So} \quad \left.\begin{array}{l} u(\infty) = a\sqrt{\pi}\,C_1 + C_2 = 1 \\ u(-\infty) = -a\sqrt{\pi}\,C_1 + C_2 = -1 \end{array}\right\} \Rightarrow C_2 = 0, \; C_1 = \frac{1}{a\sqrt{\pi}}$$

$\xi \to -\xi$

Specific solution $$\psi(x,t) = \frac{1}{a\sqrt{\pi}} \int_0^{x/\sqrt{t}} e^{-\xi^2/4a^2} d\xi = \frac{2}{\sqrt{\pi}} \int_0^{x/2a\sqrt{t}} e^{-v^2} dv =$$

$$= \operatorname{erf}\left(\frac{x}{2a\sqrt{t}}\right) \quad \text{Gauss' error function}$$

Generate new solutions to adapt to boundary conditions by differentiation (possible for PDE's with constant coefficients)

since $\frac{\partial}{\partial x}\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x \partial t} = \frac{\partial^2 \psi}{\partial t \partial x} = \frac{\partial}{\partial t}\left(\frac{\partial \psi}{\partial x}\right)$ and $\frac{\partial}{\partial x}\left(a^2 \frac{\partial^2 \psi}{\partial x^2}\right) =$

$= a^2 \frac{\partial^3 \psi}{\partial x^3} = a^2 \frac{\partial^2}{\partial x^2}\left(\frac{\partial \psi}{\partial x}\right)$ so $\frac{\partial \psi}{\partial x}$ (and $\frac{\partial^2 \psi}{\partial x^2}$) is also solution

Differentiate the $\psi(x,t)$ above:

$$\frac{\partial \psi}{\partial x} = \frac{2}{\sqrt{\pi}} \frac{\partial}{\partial x} \int_0^{x/2a\sqrt{t}} e^{-v^2} dv = \frac{1}{a\sqrt{\pi t}} e^{-x^2/4a^2 t} \equiv \psi_1(x,t)$$

Differentiate again: $\psi_2(x,t) = \dfrac{x}{2a^3\sqrt{t^3\pi}}\, e^{-x^2/4a^2t}$

The solutions still need to be adapted to boundary conditions

Another method: translate a solution and integrate over the translation parameter $\psi_1(x,t) \rightarrow \psi_1(x-\alpha, t)$

$$\psi(x,t) = \frac{1}{2a\sqrt{\pi t}} \int_{-\infty}^{\infty} C(\alpha)\, e^{-(x-\alpha)^2/4a^2t}\, d\alpha \qquad \text{set } \xi = \frac{x-\alpha}{2a\sqrt{t}},\ \alpha = x - 2a\xi\sqrt{t}$$

$$d\alpha = -2a\sqrt{t}\, d\xi$$

$$\Rightarrow \psi(x,t) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} C(x - 2a\xi\sqrt{t})\, e^{-\xi^2}\, d\xi$$

Setting $t=0 \rightarrow C(x)$ independent of ξ and with $\int_{-\infty}^{\infty} e^{-\xi^2} d\xi = \sqrt{\pi}$ we have $\psi(x,0) = C(x)$ or $C(x) = \psi_0(x)$ initial distribution

So $$\psi(x,t) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \psi_0(x - 2a\xi\sqrt{t})\, e^{-\xi^2}\, d\xi$$

The initial distribution spreads out over time and is damped by the Gaussian weight function $e^{-\xi^2}$

Application: Infinite system with initially $\psi_0 = 0$ $|x| \geq 1$ and $\psi_0 = 1$ for $|x| < 1$. The range of ψ_0 in terms of ξ is found from $x - 2a\xi\sqrt{t} = \pm 1$ so we obtain

$$\psi(x,t) = \frac{1}{\sqrt{\pi}} \int_{(x-1)/2a\sqrt{t}}^{(x+1)/2a\sqrt{t}} e^{-\xi^2}\, d\xi = \frac{1}{2}\left\{ \mathrm{erf}\left(\frac{x+1}{2a\sqrt{t}}\right) - \mathrm{erf}\left(\frac{x-1}{2a\sqrt{t}}\right) \right\}$$