.

1B METHODS LECTURE NOTES

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PART IV:

PDEs on unbounded domains

9 CHARACTERISTICS

9.1 Well-posed problems

In chapters 3,4,5 our development of PDEs on bounded domains was based largely on physical considerations, not just in the origin of the equations themselves, but also in motivating the various kinds of BCs and ICs that are necessary and sufficient to guarantee a unique solution.

- For the 1D wave equation on a finite string we specified the boundary values y(0,t) and y(L,t) for all t as well as the initial displacement y(x,0) and initial velocity $y_t(x,0)$.
- For the heat equation in a finite bar for temperature distribution $\theta(x,t)$ we specified the boundary values $\theta(0,t)$ and $\theta(L,t)$ and the initial distribution $\theta(x,0)$ but not the initial time derivative.
- For the Laplace equation (e.g. for steady heat conduction) all that was required was the boundary value. More generally for the Laplace equation on a domain \mathcal{D} with boundary $\partial \mathcal{D}$ (in 1D, 2D or 3D) the following is standard terminology: solve for ϕ throughout \mathcal{D} with –

Dirichlet problem: ϕ being specified on the boundary $\partial \mathcal{D}$;

Neumann problem: the normal derivative \underline{n} . $\nabla \phi$ being specified on the boundary. It can be shown that the Dirichlet problem has a unique solution whereas the solution of the Neumann problem is unique up to just an additive constant.

This illustrates that the exact nature of data that is necessary and sufficient for a unique solution depends non-trivially on the kind of equation being considered. Also if the equation is just viewed mathematically in terms of all its independent variables (without identifying space or time) then an IC is just another kind of BC (for the variable t). If we have a PDE for ϕ with auxiliary data (values of ϕ and its derivatives) specified on some surface (e.g. along a line in 2D or on a surface in 3D) then this data is called **Cauchy data** and the problem is called a **Cauchy problem**.

In generality, a **problem** comprises a PDE plus some auxiliary data. The problem is said to be **well-posed** (in the sense of Hadamard) if three conditions hold:

(WP1): a solution exists;

(WP2): the solution is unique;

(WP3): the solution depends continuously on the auxiliary data. (Intuitively speaking a small change in the data should result in a small change in the full solution; but a rigorous statement of this condition requires a notion of nearness (topology) and continuity in spaces of functions, which we don't develop in this course).

So far we have always considered well-posed problems. Note that (WP1) can be violated if we attempt to impose too many auxiliary conditions and (WP2), if we don't make enough demands on the solution. (WP3) is an interesting additional requirement, motivated again by physical considerations – since physical systems cannot be measured or set up with infinite precision, we would want the solution to be suitably stable under small perturbations of the data, if the equation is to usefully model the physical situation. (But the mathematical subject of *chaos theory* studies precisely the opposite behaviour!)

Example. An intuitive example of an ill-posed problem that satisfies (WP1) and (WP2) but not (WP3) is the "backwards-in-time" heat equation. Consider the heat equation for u(x,t) on $0 \le x \le L$ with BCs specified at x=0,L. Usually we specify an IC of u at t=0. Diffusion is a "smoothing" process so we expect that small perturbations in u(x,0) will not grow, and the problem is indeed well-posed. But suppose instead we specify u(x,T) at some (late) time T and ask for u(x,0) at an earlier time t=0 say. This problem can be shown to violate (WP3) – intuitively if u(x,0) has a complex detailed structure e.g. with high spatial gradients, they will be quickly smoothed out by heat flow gradients and tend to leave only a small imprint on u(x,T) at the later time T i.e. small perturbations in the latter will back-evolve into large changes in the former. Note also that if (as physically usual) we have an asymptotic steady state, all initial conditions will evolve to become very close to it, and hence remain encoded only in arbitrarily small perturbations of the steady state.

Example. (An ill-posed Laplace equation problem).

Consider the following problem – we have Laplace's equation $u_{xx} + u_{yy} = 0$ on the upper half plane $y \ge 0$ and $-\infty < x < \infty$, with BCs

$$u(x, 0) = f(x)$$
 and $u_y(x, 0) = g(x)$

where f and g are specified functions. If $f(x) = f_1(x) = 0$ and $g(x) = g_1(x) = 0$ then we have the solution $u_1(x, y) = 0$ which can be shown to be unique.

If now we set $f(x) = f_2(x) = 0$ and $g(x) = g_2(x) = \frac{\sin Ax}{A}$ then again we have a unique solution (which can be found by looking for a separated variable solution u(x,y) = X(x)Y(y) etc.) given by

$$u_2(x,y) = \frac{\sin Ax \, \sinh Ay}{A^2}.$$

Now if we consider $A \to \infty$ we have $f_2 \to f_1$ (actually they're equal) and $g_2 \to g_1$ but $|u_1 - u_2|$ can become arbitrarily large e.g. at $x = \pi/(2A)$ we have $u_2(x, y) = (\sinh Ay)/A^2 \approx e^{Ay}/A^2 \to \infty$ as $A \to \infty$. Hence the problem is ill-posed.

9.2 Characteristics for first order PDEs

We consider the general 1st order linear (actually so-called quasi-linear because of RHS dependence on u) PDE in 2D :

$$\alpha(x,y)u_x + \beta(x,y)u_y = \gamma(x,y,u) \tag{1}$$

(where the subscripts denote partial derivatives), together with Cauchy data specifying u(x,y) along a specified "initial" curve B in the xy plane. B will be described parametrically (parameter t):

$$x = x^B(t) y = y^B(t)$$

and u along this curve is a specified function h(t):

$$u(x^B(t), y^B(t)) = h(t).$$

The homogeneous case $\gamma = 0$

Consider first the homogeneous case $\gamma = 0$ in eq. (1)

$$\alpha u_x + \beta u_y = 0. (2)$$

Introducing the vector field $\underline{A}(x,y) = (\alpha(x,y), \beta(x,y))$ (depending on the PDE but not the Cauchy data) we see that eq. (2) is

$$\underline{A}.\nabla u = 0. \tag{3}$$

Interlude: facts about parameterised curves and vector fields

- (a) if $(x = x^C(s), y = y^C(s))$ is any parameterised curve C, its tangent vector at point labelled by s is $\underline{T} = (dx^C/ds, dy^C/ds)$.
- (b) if u(x,y) is a function on the plane, its restriction to C is $u(x^C(s), y^C(s))$ and the directional derivative along C is (by the chain rule)

$$\frac{du}{ds} = \frac{dx^C}{ds}u_x + \frac{dy^C}{ds}u_y = \underline{T}.\nabla u.$$

Hence if $T.\nabla u = 0$ (as a function of s) then u is constant along the curve C.

(c) if $\underline{A}(x,y) = (\alpha(x,y), \beta(x,y))$ is any (suitably regular) vector field on (a part of) \mathbb{R}^2 , its integral curves area 1-parameter family of non-intersecting curves filling (that part of) \mathbb{R}^2 , defined by the requirement that at any point (x,y), the curve through (x,y) has tangent $\underline{A}(x,y)$ (e.g. if we think of \underline{A} as the velocity field of a fluid then the integral curves are the flow lines of the fluid elements). More explicitly let $x = x^B(t)$ $y = y^B(t)$ be some specified curve B that is transverse to \underline{A} i.e. along B the tangent vector $(dx^B/dt, dy^B/dt)$ is nowhere parallel to \underline{A} at the same point. We then label the integral curves of \underline{A} by t, the point where they intersect B, and use parameter s along the integral curves, with s = 0 at B. Thus the t^{th} curve is x = x(t,s) y = y(t,s) (here t is a curve-label and s is the parameter along the curve) satisfying

$$\frac{dx}{ds} = \alpha(x, y) \qquad \frac{dy}{ds} = \beta(x, y) \tag{4}$$

subject to ODE initial conditions $x(t,0) = x^B(t)$ and $y(t,0) = y^B(t)$ (stating that the curves pass through B when the parameter s is 0).

Now back to our PDE

For $\alpha u_x + \beta u_y = 0$ the integral curves of the vector field (α, β) are called the **characteristic curves** of the PDE. Then eq. (3) just says that u(x,y) is constant along the characteristic curves C. Now taking B of interlude item (c) above, to be the Cauchy data curve we see that the Cauchy data values h(t) along the curve B are propagated constantly along the characteristic curves to define u(x,y) in the plane (or at least in a neighbourhood of the curve B) i.e. $u(x^C(t,s),y^C(t,s))=h(t)$ is constant in s. Finally to get an explicit expression for u(x,y) as a function of our original co-ordinates (x,y), we view the characteristic curve equations (for the t^{th} curve parameterised by s)

$$x = x^C(t, s) y = y^C(t, s)$$

as a co-ordinate transformation $(x, y) \leftrightarrow (t, s)$. If the Jacobian $J = x_t^C y_s^C - x_s^C y_t^C$ is non-zero then the transformation can be inverted, solving for (t, s) in terms of (x, y):

$$t = t(x, y) \qquad s = s(x, y)$$

and then

$$u(x,y) = h(t(x,y))$$

gives the solution of our Cauchy problem.

Note the following features of the above construction:

- (a) If any characteristic curve intersects the initial curve B more than once then the problem is over-determined the value of h(t) must then be constrained to be the same at all such multiple intersection points for a solution to exist (cf (WP1)).
- (b) If the initial curve B itself is a characteristic curve then we must have h(t) = const for a solution to exist, and in that case the solution is not unique (cf (WP2)) as it can be freely specified on all the other characteristics.
- (c) If the initial curve is transversal to all characteristics and intersects them once only, then the problem is well-posed for any h(t) and has a unique solution u(x,y) (at least in a neighbourhood of B). Note that the initial data cannot be propagated from one characteristic to another, so, for example, discontinuities in the initial data propagate along the corresponding characteristic curve.

In summary,

to solve $\alpha u_x + \beta u_y = 0$ with u(x,y) = h(t) on initial curve $(x^B(t), y^B(t))$:

(1) Write down the equations eq. (4) for the characteristics with the s=0 parameter's initial condition given by the initial curve B i.e. for each t we have the system of two ODEs:

$$\frac{dx}{ds} = \alpha$$
 $\frac{dy}{ds} = \beta$ with $x(t,0) = x^B(t)$, $y(t,0) = y^B(t)$.

- (2) Solve for the characteristics $x = x^{C}(t, s)$ $y = y^{C}(t, s)$.
- (3) Algebraically invert these relations to obtain t = t(x, y) and s = s(x, y).
- (4) Using the Cauchy data h(t) construct the solution as u(x,y) = h(t(x,y)), which represents the initial data propagated constantly along the characteristics off B.

Example. (the simplest possible example!)

Consider $u_x(x,y) = 0$ with Cauchy data u(0,y) = h(y) on the y axis. Without any fancy theory of characteristics etc., the solution to $u_x = 0$ is obviously u(x,y) = f(y) i.e. an arbitrary function of y only, and then the Cauchy data immediately gives u(x,y) = h(y). But it's instructive to identify the characteristics in this example. We have $(\alpha, \beta) = (1,0)$, a field of constant horizontal unit vectors, and initial curve B (the y axis) can be parameterised as $(x^B(t) = 0, y^B(t) = t)$ with u = h(t) along B. So the characteristics are clearly horizontal lines parallel to the x axis. Formally the tth characteristic curve goes through the point t on B viz. (x,y) = (0,t) and has

$$\frac{dx}{ds} = \alpha = 1 \qquad \frac{dy}{ds} = \beta = 0 \qquad x(0) = 0, y(0) = t$$

so $x(t,s) = s + c_1$ and $y(t,s) = c_2$, and the initial s = 0 conditions give $c_1 = 0$, $c_2 = t$ i.e. x(t,s) = s and y(t,s) = t as expected (the tth line being the horizontal line at height t). Inverting these relations gives s(x,y) = x and t(x,y) = y so u(x,y) = h(t(x,y)) = h(y) as expected.

Example. Consider

$$e^x u_x + u_y = 0$$
 with $u(x, 0) = \cosh x$.

The initial curve B is the x axis (x = t, y = 0) and the initial data along B is $h(t) = \cosh t$. We have $(\alpha, \beta) = (e^x, 1)$ so the characteristics, labelled by t, satisfy

$$\frac{dx}{ds} = e^x \qquad \frac{dy}{ds} = 1, \qquad x(0) = t \qquad y(0) = 0$$

so $e^{-x} = -s + c_1$ and $y = s + c_2$ where the integration constants depend on t via the initial conditions, which give $c_1 = e^{-t}$ and $c_2 = 0$ so $e^{-x} = e^{-t} - s$ and y = s. Inverting these expressions we get

$$s = y t = -\log(y + e^{-x})$$

and the solution to the Cauchy problem is

$$u(x,y) = h(t(x,y)) = \cosh\left[-\log(y + e^{-x})\right]$$

whose validity you can verify directly (by substitution).

9.3 Inhomogeneous problems and characteristics

For the general quasi-linear case eq. (1) viz. $\alpha(x,y)u_x + \beta(x,y)u_y = \gamma(x,y,u)$ together with u(x,y) = h(t) on curve B: $x = x^B(t)$, $y = y^B(t)$, we still have characteristic curves exactly as before (not depending on h or γ) and writing u(s) = u(x(s), y(s)) for u along any characteristic curve, eq. (1) states precisely that (for each curve labelled by t and parameterised by s):

$$\frac{du}{ds} = \gamma(x, y, u) \qquad u(0) = h(t). \tag{5}$$

Thus the only difference from our previous (homogeneous) situation is that now, u is not propagated as a constant along characteristic curves off from B, but instead we have to solve the ODE eq. (5) to obtain u(s) for each curve t i.e. to obtain u(t,s). Then just as before, we invert the relations x = x(t,s) and y = y(t,s) that define the characteristics, to get s = s(x,y) and t = t(x,y) and finally our solution is u(x,y) = u(t(x,y),s(x,y)).

Example. Consider the Cauchy problem

$$u_x + 2u_y = ye^x$$
 with $u = \sin x$ when $y = x$.

Thus $\alpha = 1$, $\beta = 2$ $\gamma = ye^x$ and the initial curve B is (x = t, y = t), with initial data $h(t) = \sin t$. We first solve for the characteristic curves:

$$\frac{dx}{ds} = 1 \qquad \frac{dy}{ds} = 2, \qquad x(0) = t \ y(0) = t$$

giving x = s + t and y = 2s + t. Thus along the tth characteristic curve we have

$$\frac{du}{ds} = \gamma(x, y, u) = ye^x = (2s + t)e^{s+t} \quad \text{with } u(0) = h(t) = \sin t.$$

The solution is (exercise, but remember that t is just a parameter!)

$$u(s,t) = (2-t)e^t + \sin t + e^{s+t}(t+2s-2). \tag{6}$$

Next inverting the characteristic curve equations gives

$$s = y - x \qquad \quad t = 2x - y$$

and substituting into eq. (6) gives the solution

$$u(x,y) = (2 - 2x + y)e^{2x-y} + \sin(2x - y) + e^{x}(y - 2).$$

9.4 Classification of second order linear PDEs

We can usefully generalise the idea of characteristics to apply to some classes of second order PDEs. Consider the general second-order linear PDE (in two variables)

$$a(x,y)u_{xx} + 2b(x,y)u_{xy} + c(x,y)u_{yy} + d(x,y)u_x + e(x,y)u_y + f(x,y)u = g(x,y)$$
 (7)

with Cauchy data u = h(t), $u_x = m(t)$, $u_y = n(t)$ specified along some curve B given parametrically as $x = x^B(t)$, $y = y^B(t)$. Note that if we differentiate u along t we get

$$h'(t) = \frac{dx^B}{dt}u_x + \frac{dy^B}{dt}u_y = \frac{dx^B}{dt}m(t) + \frac{dy^B}{dt}n(t)$$

giving a relation between h, m and n. Hence no more than two of these functions can be freely specified.

In terms of the coefficient functions for the second derivatives (and note the conventionally used extra factor of 2 in the u_{xy} term), we introduce the following classification of linear 2^{nd} order PDEs. This will be significant for the behaviour of solutions, and especially for their relation to the Cauchy data, via an associated notion of characteristic curves. The equation (7) is called:

- hyperbolic if $b^2 ac > 0$.
- parabolic if $b^2 ac = 0$,
- elliptic if $b^2 ac < 0$.

Note that the wave equation is hyperbolic $(c = 1, b = 0, a = \text{-wave speed}^2)$, the diffusion equation is parabolic (a = 0, b = 0, c = -D) and the Laplace equation is elliptic (a = c = 1, b = 0).

Note that in general, a, b and c are functions of (x, y) so a single equation can be hyperbolic, parabolic and elliptic in different parts of the plane.

Now consider introducing new independent variables ξ, η by the substitution

$$\xi = \phi(x, y)$$
 $\eta = \psi(x, y)$

transforming the equation into one of the same type:

$$A(\xi,\eta)u_{\xi\xi} + 2B(\xi,\eta)u_{\xi\eta} + C(\xi,\eta)u_{\eta\eta} + \dots = G(\xi,\eta).$$

The substitution is straightforward but cumbersome to calculate. For example we have $u_x = u_\xi \phi_x + u_\eta \psi_x$ so

$$u_{xx} = [u_{\xi\xi}\phi_x + u_{\xi\eta}\psi_x] \phi_x + u_{\xi}\phi_{xx} + [u_{\eta\xi}\phi_x + u_{\eta\eta}\psi_x] \psi_x + u_{\eta}\psi_{xx}$$

etc. and in particular we get the new 2nd derivative coefficients to be

$$A = a\phi_x^2 + 2b\phi_x\phi_y + c\phi_y^2$$

$$B = a\phi_x\psi_x + b(\phi_x\psi_y + \phi_y\psi_x) + c\phi_y\psi_y$$

$$C = a\psi_x^2 + 2b\psi_x\psi_y + c\psi_y^2.$$

Note that A (and/or C) can be made zero if ϕ (and/or ψ) can be chosen to satisfy

$$a\phi_x^2+2b\phi_x\phi_y+c\phi_y^2=0$$
 i.e.
$$aM^2+2bM+c=0\quad\text{for}\quad M=\phi_x/\phi_y$$
 i.e.
$$M=\frac{-b\pm\sqrt{b^2-ac}}{a}.$$

In that case the corresponding co-ordinate curves $\xi = \phi(x, y) = \text{const}$ (and/or $\eta = \psi(x, y) = \text{const}$) are called **characteristic curves** of the original PDE. Note that if $\phi(x, y) = \text{const}$ defines a curve y = y(x) then

$$\phi_x + \phi_y \frac{dy}{dx} = 0$$
 so $\frac{dy}{dx} = -\frac{\phi_x}{\phi_y}$.

Hence in terms of a, b and c the characteristic curves are given by solving

$$\frac{dy}{dx} = -\left[\frac{-b \pm \sqrt{b^2 - ac}}{a}\right]$$

(obtaining the solution in the form f(x,y) = const and then using f for ϕ or ψ .)

For *elliptic equations* there are *no* real characteristics.

For parabolic equations we get a single family of characteristics $\frac{dy}{dx} = \frac{b}{a}$.

For hyperbolic equations we get two families of characteristics corresponding to the two roots

$$M_{\pm} = \frac{-b \pm \sqrt{b^2 - ac}}{a}$$

and using the corresponding change of variables

$$\xi = \phi(x, y)$$
 $\eta = \psi(x, y)$

with co-ordinate lines being the characteristic curves, the hyperbolic equation takes the form

$$u_{\xi\eta} + D(\xi, \eta)u_{\xi} + E(\xi, \eta)u_{\eta} + F(\xi, \eta)u = G(\xi, \eta)$$

having no $u_{\xi\xi}$ or $u_{\eta\eta}$ term, which is called the **canonical form of the hyperbolic equation**.

Example. The equation $u_{yy} - xyu_{xx} = 0$ has a = -xy, b = 0 and c = 1 so $b^2 - ac = xy$ so the equation is hyperbolic in the first (x > 0, y > 0) and third (x < 0, y < 0) quadrants, elliptic in the second and fourth quadrants and parabolic along the axes x = 0 or y = 0. In the hyperbolic region we have

$$\frac{-b \pm \sqrt{b^2 - ac}}{a} = \pm \frac{1}{\sqrt{xy}}$$

so the two families of characteristics are given by

$$\frac{dy}{dx} = \pm \frac{1}{\sqrt{xy}}$$
 i.e. $\frac{y^{3/2}}{3} \pm x^{1/2} = c$

and the substitution

$$\xi = \frac{y^{3/2}}{3} + x^{1/2}$$
 $\eta = \frac{y^{3/2}}{3} - x^{1/2}$

(after a lengthy but straightforward calculation, that we omit!) will reduce the equation to canonical form in the hyperbolic region.

9.5 D'Alembert's general solution of the wave equation

An especially important example of a hyperbolic equation and its characteristics is the (1D) wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \quad \text{with } u(x,0) = \phi(x), \ u_t(x,0) = \psi(x)$$

which is hyperbolic in the whole (x,t) plane. The characteristics are easily calculated to be $x \pm ct = \text{const}$ so we introduce new variables

$$\xi = x + ct$$
 $\eta = x - ct$

and the equation takes an especially simple canonical form

$$\frac{\partial^2 u}{\partial \xi \partial \eta} = 0.$$

The general solution is easily obtained by first integrating w.r.t. ξ giving $\partial u/\partial \eta = F(\eta)$ and then

$$u = \int_{-\eta}^{\eta} F(y)dy + g(\xi) = f(\eta) + g(\xi)$$
(8)

for arbitrary functions f and g ($g(\xi)$ being the η -integration constant for each ξ).

Thus the solution is the sum of two terms that are constant respectively on the two families of characteristics. Let us now impose our initial conditions on the general solution eq. (8). At t = 0 (recalling that $\xi, \eta = x \pm ct$) we get

$$u(x,0) = f(x) + g(x) = \phi(x)$$

 $u_t(x,0) = -cf'(x) + cg'(x) = \psi(x).$

Differentiating the first equation then gives with the second equation:

$$g'(x) = \frac{1}{2} \left[\phi'(x) + \frac{1}{c} \psi(x) \right]$$

SO

$$g(x) = \frac{1}{2}(\phi(x) - \phi(0)) + \frac{1}{2c} \int_0^x \psi(y) \, dy$$

$$f(x) = \frac{1}{2}(\phi(x) + \phi(0)) - \frac{1}{2c} \int_0^x \psi(y) \, dy$$

and we obtain the very elegant d'Alembert's solution of the wave equation:

$$u(x,t) = f(x-ct) + g(x+ct)$$

$$= \frac{1}{2} [\phi(x+ct) + \phi(x-ct)] + \frac{1}{2c} \int_{x-ct}^{x+ct} \psi(y) \, dy.$$
 (9)

We see that u(x,t) is determined fully by the values of the initial functions ϕ , ψ in the interval [x-ct,x+ct] of the x-axis, whose endpoints are cut out by the characteristics through the point (x,t). This interval is called the **domain of dependence** for the solution at (x,t).

Conversely the initial data at the point $(\xi, 0)$ of the x-axis at time t = 0 influences u(x, t) at points (x, t) in the wedge-shaped region bounded by the characteristics $x \pm ct = \xi$ through $(\xi, 0)$ i.e. the region $\xi - ct < x < \xi + ct$. Thus disturbances or signals travel only with speed c.

In particular, discontinuities in the initial data ϕ propagate along characteristics. For example consider $\phi(x) = H(x)$ and $\psi(x) = 0$. Then $u(x,t) = \frac{1}{2} [H(x-ct) + H(x+ct)]$ which is an initial (t=0) unit step discontinuity at x=0 simply propagating to the left and right at speeds $\pm c$, each with half unit heights.

10 Green's functions for PDEs

In this final chapter we will apply the idea of Green's functions to PDEs, enabling us to solve the wave equation, diffusion equation and Laplace equation in unbounded domains, and also with forcing terms (i.e. inhomogeneous PDEs). In some of these developments, the Fourier transform will play a key role (via the "differentiation becomes multiplication" rule) and to each of our equations we will associate a fundamental FT pair and a corresponding so-called **fundamental solution**.

10.1 FTs for the diffusion equation

Consider the Cauchy problem for the 1D diffusion equation

$$\frac{\partial \theta}{\partial t} = D \frac{\partial^2 \theta}{\partial x^2}$$
 $\theta(x,0) = f(x)$

and $\theta \to 0$ as $|x| \to \infty$ (e.g. diffusion of heat in an infinitely long bar with initial temperature f(x)). Taking FTs of the diffusion equation w.r.t. x and writing the FT of $\theta(x,t)$ as $\tilde{\theta}(k,t)$ we have

$$\frac{\partial}{\partial t}\tilde{\theta}(k,t) = -Dk^2\tilde{\theta}(k,t) \qquad \tilde{\theta}(k,0) = \tilde{f}(k)$$

and a simple t integration (using the initial condition) gives

$$\tilde{\theta}(k,t) = \tilde{f}(k) e^{-Dtk^2}.$$
(10)

To apply the convolution theorem (to invert the RHS product in eq. (10)) we need to identify the function g(x,t) such that

$$\tilde{g}(k,t) = e^{-Dtk^2}$$

i.e. we want the inverse FT of a Gaussian. On exercise sheet 3 question 9 you've already derived the FT pair for a general Gaussian viz.

$$\phi(x) = e^{-a^2x^2} \leftrightarrow \tilde{\phi}(k) = \frac{\sqrt{\pi}}{a}e^{-\frac{k^2}{4a^2}}.$$

Hence identifying $1/4a^2$ as Dt and rescaling by $\sqrt{\pi}/a$ we get the fundamental Fourier transform pair for the diffusion equation

$$g(x,t) = \frac{1}{\sqrt{4\pi Dt}} e^{\frac{-x^2}{4Dt}} \iff \tilde{g}(k,t) = e^{-Dk^2t}, \tag{11}$$

and so, using the convolution theorem, the general solution to our Cauchy problem is

$$\theta(x,t) = \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} f(u) \, e^{-\frac{(x-u)^2}{4Dt}} \, du = \int_{-\infty}^{\infty} f(u) \, S_d(x-u,t) \, du, \tag{12}$$

where the function $S_d(x-u,t)$ is called the **fundamental solution** or the **source function** for the diffusion equation. Here it is associated with the *unforced (homogeneous)* equation with *inhomogeneous* ICs, but below we will see that it arises also in the solution of the *forced (inhomogeneous)* equation with *homogeneous* ICs.

The Gaussian pulse as IC

Suppose the IC for the heat equation is the Gaussian

$$f(x) = \sqrt{\frac{a}{\pi}} \theta_0 e^{-ax^2}$$

normalised so that

$$\int_{-\infty}^{\infty} f(x) \, dx = \theta_0.$$

Substituting into eq. (12) we obtain

$$\theta(x,t) = \frac{\theta_0 a^{1/2}}{\sqrt{4\pi^2 Dt}} \int_{-\infty}^{\infty} \exp\left[-au^2 - \frac{(x-u)^2}{4Dt}\right] du$$

$$= \frac{\theta_0 a^{1/2}}{\sqrt{4\pi^2 Dt}} \int_{-\infty}^{\infty} \exp\left[\frac{-([1+4aDt]u^2 - 2xu + x^2)}{4Dt}\right] du$$

$$= \frac{\theta_0 a^{1/2} \exp\left[-\frac{ax^2}{1+4aDt}\right]}{\sqrt{4\pi^2 Dt}}$$

$$\times \int_{-\infty}^{\infty} \exp\left[\frac{-(1+4aDt)}{4Dt} \left(u - \frac{x}{1+4aDt}\right)^2\right] du,$$

$$= \theta_0 \exp\left[-\frac{ax^2}{1+4aDt}\right] \frac{1}{\sqrt{4\pi^2 Dt}} \sqrt{\frac{4aDt}{1+4aDt}} \int_{-\infty}^{\infty} e^{-v^2} dv$$

where we have used the substitution

$$v = \sqrt{\frac{1 + 4aDt}{4Dt}} \left(u - \frac{x}{1 + 4aDt} \right) \qquad du = \sqrt{\frac{4Dt}{1 + 4aDt}} dv.$$

Thus finally

$$\theta(x,t) = \theta_0 \sqrt{\frac{a}{\pi(1+4aDt)}} \exp\left[-\frac{ax^2}{1+4aDt}\right].$$

Thus an initial Gaussian retains a Gaussian form, with its squared width (1 + 4aDt)/a spreading linearly with t (recall linear growth of variance for diffusing probabilistic processes) while the total area remains constant (cf conservation law of diffusing material that is built in to the diffusion equation) and the peak at x = 0 drops as $t^{-1/2}$. These features are illustrated in the figure.

The delta function pulse as IC

If the IC for the diffusion equation is the delta function

$$f(x) = \theta_0 \delta(x)$$

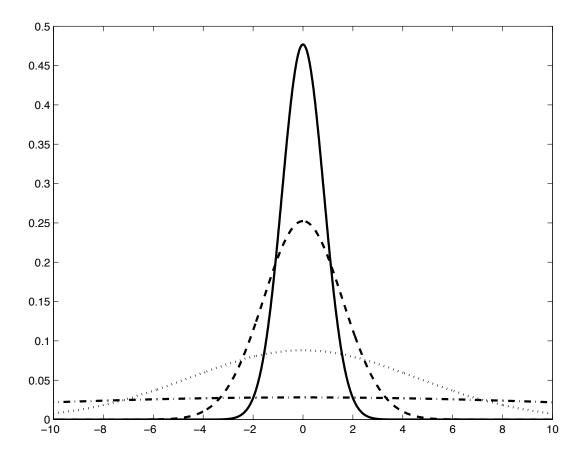


Figure 1: Plots (with $a=D=1=\theta_0$) of the Gaussian pulse solution for: t=0.1 (solid line); t=1 (dashed); t=10 (dotted); and t=100 (dot-dashed).

then substitution into eq. (12) and the sampling property of $\delta(x)$ gives

$$\theta = \frac{\theta_0}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} \delta(u) \exp\left[\frac{-(x-u)^2}{4Dt}\right] du \tag{13}$$

$$= \frac{\theta_0}{\sqrt{4\pi Dt}} \exp\left[\frac{-x^2}{4Dt}\right] = \theta_0 S_d(x, t), \tag{14}$$

i.e. the solution is the source function itself. Thus for all t > 0 the δ -pulse spreads as a Gaussian and as $t \to 0$ from above, we regain the δ function as a Gaussian in the limit of zero width while keeping the area constant (and hence unbounded height).

Note also the ubiquitous appearance of the dimensionless group $\eta^2 = \frac{x^2}{4Dt}$ that we previously introduced (in chapter 4) as the so-called similarity variable.

10.2 The forced heat equation

Consider the forced 1D heat equation on an infinite domain, with homogeneous BCs

$$\frac{\partial}{\partial t}\theta_f(x,t) - D\frac{\partial^2}{\partial x^2}\theta_f(x,t) = f(x,t) \qquad \theta_f(x,0) = 0, \tag{15}$$

(with subscript 'f' for 'forced').

Remark. In the previous section we solved the homogeneous equation with inhomogeneous BCs and here we are considering the forced (inhomogeneous) equation with homogeneous BCs. For the general case of the forced equation with inhomogeneous BCs we can reduce the problem to these two cases, writing the solution as $y = y_h + y_f$ where y_h satisfies the homogeneous equation with the given inhomogeneous BCs and y_f satisfies the forced equation with homogeneous BCs. This decomposition will clearly apply to our other equations as well. \Box

To solve the problem of eq. (15) we seek a Green's function $G(x,t;\xi,\tau)$ such that

$$\frac{\partial}{\partial t}G(x,t;\xi,\tau) - D\frac{\partial^2}{\partial x^2}G(x,t;\xi,\tau) = \delta(x-\xi)\delta(t-\tau), \qquad G(x,0;\xi,\tau) = 0, (16)$$

because then (formally at least)

$$\theta_f(x,t) = \int_0^\infty \int_{-\infty}^\infty G(x,t;\xi,\tau) f(\xi,\tau) d\xi d\tau,$$

when substituted into the heat equation (using a double application of the sampling property of delta functions) will satisfy eq. (15).

Taking FTs of eq. (16) w.r.t. x (and recalling that the FT of $\delta(x-\xi)$ is $e^{-ik\xi}$) we obtain (after multiplying through by e^{Dk^2t})

$$\begin{split} \frac{\partial}{\partial t} \left[e^{Dk^2t} \tilde{G}(k,t;\xi,\tau) \right] &= e^{-ik\xi + Dk^2t} \delta(t-\tau), \qquad \tilde{G}(k,0;\xi,\tau) = 0, \\ e^{Dk^2t} \tilde{G}(k,t;\xi,\tau) &= e^{-ik\xi} \int_0^t e^{Dk^2u} \delta(u-\tau) \, du. \end{split}$$

so by the sampling property, the remaining integral is zero if $t < \tau$, and is equal to $e^{Dk^2\tau}$ if $t > \tau$. Thus

$$\begin{split} \tilde{G}(k,t;\xi,\tau) &= H(t-\tau)e^{-ik\xi}e^{-Dk^2(t-\tau)} \\ G(x,t;\xi,\tau) &= \frac{H(t-\tau)}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-\xi)}e^{-Dk^2(t-\tau)} \, dk \\ &= \frac{H(t')}{2\pi} \int_{-\infty}^{\infty} e^{ikx'}e^{-Dk^2t'} \, dk \end{split}$$

where we have written $x' = x - \xi$ and $t' = t - \tau$. But now we have just recovered the Gaussian function written in the FT pair eq. (11) (with variables x', t') and so we immediately get

$$G(x,t;\xi,\tau) = \frac{H(t-\tau)\exp\left[\frac{-(x-\xi)^2}{4D(t-\tau)}\right]}{\sqrt{4\pi D(t-\tau)}}$$

$$= H(t-\tau)S_d(x-\xi,t-\tau). \tag{18}$$

Note that this involves the *same* source function

$$S_d(x,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left[-\frac{x^2}{4Dt}\right]$$

that we encountered in the solution of the *homogeneous* equation with *inhomogeneous* ICs viz. eq.(12).

Duhamel's principle

Duhamel's principle asserts a relationship between (a) the solution of a forced equation with homogeneous ICs, and (b) the solution of the unforced (homogeneous) equation with non-homogeneous ICs. Let us recall our solution for (b) as given in eq. (12) with a slight generalisation – let us take our initial data at time $t = \tau$ (instead of t = 0) and solve for $t > \tau$. A simple time translation of eq. (12) gives the solution of

$$\theta_t - D\theta_{xx} = 0$$
 with $\theta(x, \tau) = g(x)$

to be

$$\theta(x,t) = \int_{-\infty}^{\infty} g(u)S_d(x-u,t-\tau) du \qquad t > \tau$$
 (19)

i.e. the initial data g(x) at $t = \tau$ has been propagated for a time $t - \tau$ up to time t.

Now consider our solution of the forced problem obtained above viz. the problem

$$\theta_t - D\theta_{xx} = f(x, t)$$
 with $\theta(x, 0) = 0$

having solution

$$\theta_f(x,t) = \int_0^t \left[\int_{-\infty}^\infty f(u,\tau) S_d(x-u,t-\tau) du \right] d\tau.$$
 (20)

If we view the forcing term f(x,t) for each fixed time $t=\tau$ as an IC(!) at initial time $t=\tau$ then the integral in the square brackets represents its effect propagated to time t via eq. (19). Then the time integral in eq. (20) expresses the forced solution θ_f as the accumulation (superposition) of all these IC effects from all times τ earlier than t, propagated for time interval $t-\tau$ up to time t. The upper limit t of this integral is a causality effect (expressed in the Green's function by the $H(t-\tau)$ factor) – an IC applied at a time τ cannot influence the past $t < \tau$, but contributes to the solution only for all later times $t > \tau$.

10.3 The forced wave equation

Consider the forced 1D wave equation with homogeneous ICs:

$$\frac{\partial^2 y_f}{\partial t^2} - c^2 \frac{\partial^2 y_f}{\partial x^2} = f(x, t)$$

$$y_f(x, 0) = 0, \quad \frac{\partial y_f}{\partial t}(x, 0) = 0$$
(21)

with $-\infty < x < \infty$ and $t \ge 0$. As before we seek a Green's function $G(x,t;\xi,\tau)$ satisfying

$$\frac{\partial^2}{\partial t^2} G(x, t; \xi, \tau) - c^2 \frac{\partial^2}{\partial x^2} G(x, t; \xi, \tau) = \delta(x - \xi) \delta(t - \tau),$$

$$G(x, 0; \xi, \tau) = 0, \frac{\partial}{\partial t} G(x, 0; \xi, \tau) = 0$$
(22)

so then

$$y_f(x,t) = \int_0^\infty \int_{-\infty}^\infty f(\xi,\tau) G(x,t;\xi,\tau) \,d\xi \,d\tau \tag{23}$$

will be a solution of eq. (21).

Taking FTs with respect to x (and wlog taking c > 0) we get

$$\frac{\partial^2}{\partial t^2} \tilde{G}(k,t;\xi,\tau) + k^2 c^2 \tilde{G}(k,t;\xi,\tau) = e^{-ik\xi} \delta(t-\tau).$$

with both \tilde{G} and $\partial \tilde{G}/\partial t$ being zero at t=0.

Now we recognise this as an ODE Green's function problem for an IVP, essentially the same as the example given previously at the end of section 7.3 – the latter example just needs to be slightly generalised by introducing the constant k^2c^2 and the scale factor $e^{-ik\xi}$ to multiply $\delta(t-\tau)$ on RHS. Thus the solution is:

$$\tilde{G}(k,t;\xi,\tau) = \frac{e^{-ik\xi} \sin[kc(t-\tau)]H(t-\tau)}{kc}.$$

To invert this FT we use Dirichlet's discontinuous formula (in the last line below) to get:

$$G(x,t;\xi,\tau) = \frac{H(t-\tau)}{2\pi c} \int_{-\infty}^{\infty} \frac{e^{ik(x-\xi)}\sin[kc(t-\tau)]}{k} dk,$$

$$= \frac{H(t-\tau)}{\pi c} \int_0^\infty \frac{\cos[k(x-\xi)] \sin[kc(t-\tau)]}{k} dk,$$

$$= \frac{H(t-\tau)}{2\pi c} \int_0^\infty \frac{\sin[k(x-\xi+c[t-\tau])]}{k} dk$$

$$-\frac{H(t-\tau)}{2\pi c} \int_0^\infty \frac{\sin[k(x-\xi-c[t-\tau])]}{k} dk$$

$$= \frac{H(t-\tau)}{4c} \left\{ \operatorname{sgn}(x-\xi+c[t-\tau]) - \operatorname{sgn}(x-\xi-c[t-\tau]) \right\}.$$

Note that the $H(t-\tau)$ factor imposes $t-\tau>0$ and we can simplify the above formula using the following

Exercise: Suppose that B > 0. Then

$$\operatorname{sgn}(A+B) - \operatorname{sgn}(A-B) = 2H(B-|A|).$$

(Just consider the cases A > B, A < -B and -B < A < B separately.) \square

Thus we get the **causal fundamental solution** of the wave equation

$$G(x,t;\xi,\tau) = \frac{H(c(t-\tau) - |x-\xi|)}{2c}.$$
 (24)

(Note that this expression already requires $t-\tau>0$ for G to be non-zero so we need not include the $H(t-\tau)$ factor, which is redundant.)

We see that G is non-zero only when $|x - \xi| < c(t - \tau)$ so a forcing disturbance $f(\xi, \tau)$ at position ξ and time τ can affect a point at x only for times $t > \tau + |x - \xi|/c$ i.e. we have a a finite speed c of propagation of disturbances.

Using our Green's function, the solution (21) is now

$$y_f(x,t) = \frac{1}{2c} \int_0^t \int_{x-c(t-\tau)}^{x+c(t-\tau)} f(\xi,\tau) \, d\xi \, d\tau.$$
 (25)

Notice that the order of integration in this case is important, correctly capturing the τ -dependent domain of influence of the forcing i.e. the ξ limits depending on τ .

Exercise. (Duhamel's principle for the wave equation).

Recalling D'Alembert's solution eq. (9) of the unforced (homogeneous) wave equation with non-homogeneous ICs, note that

$$I(x,t) = \frac{1}{2c} \int_{x-c(t-\tau)}^{x+c(t-\tau)} f(\xi,\tau) d\xi \qquad t > \tau$$

is the D'Alembert solution with initial data given at time τ : $u(x,\tau) = 0$ $u_t(x,\tau) = f(x,\tau)$. Hence the solution eq. (25) of the forced equation with homogeneous initial data can again be viewed as a superposition of influences from the forcing term $f(x,\tau)$ used as an IC (here an IC for the time derivative) for each $\tau < t$.

10.4 Poisson's equation

Poisson's equation is the forced Laplace equation:

$$\nabla^2 u = -f(\mathbf{x}) \tag{26}$$

and we will consider it in domains \mathcal{D} (possibly infinite) in 2 and 3 space dimensions \mathbf{x} with suitable BCs (cf. later). We will approach its solution by establishing a notion of Green's function for it. Unlike the diffusion and wave equations, we have no time co-ordinate and correspondingly no causality constraint. We will also encounter other differences, making its solution via Green's functions less straightforward than that of the latter two equations. We'll use a generalisation of the delta function to more than one dimension. The natural generalisation, denoted $\delta(\mathbf{r} - \mathbf{r}_0)$ is deemed to have the following properties:

$$\delta(\mathbf{r} - \mathbf{r}_0) = 0, \ \forall \mathbf{r} \neq \mathbf{r}_0, \ \int_{\mathcal{D}} \delta(\mathbf{r} - \mathbf{r}_0) d\mathbf{r} = \begin{cases} 1 & \mathbf{r}_0 \in \mathcal{D} \\ 0 & \text{otherwise,} \end{cases}$$
 (27)

and the sampling property

$$\int_{\mathcal{D}} f(\mathbf{r}) \, \delta(\mathbf{r} - \mathbf{r}_0) \, dV = f(\mathbf{r}_0) \quad \text{if } \mathbf{r}_0 \in \mathcal{D}.$$

The integration is over either a part of \mathbb{R}^2 or \mathbb{R}^3 and then dV denotes respectively the surface of volume element.

The free-space Green's function

The **fundamental solution** to Poisson's equation is defined to be the solution to the problem

$$\nabla^2 G(\mathbf{r}; \mathbf{r}_0) = \delta(\mathbf{r} - \mathbf{r}_0).$$

Since the problem rotationally symmetric (in 2D or 3D) about the special point \mathbf{r}_0 , the fundamental solution can only depend on the scalar distance from that point:

$$G(\mathbf{r}; \mathbf{r}_0) = G(|\mathbf{r} - \mathbf{r}_0|) = G(r).$$

Let us write G_3 and G_2 for this function in 3D and 2D respectively.

Integrating over a sphere (in 3D) or circle (in 2D) of radius r centred at \mathbf{r}_0 we obtain

$$\int_{V} \nabla^{2} G_{3}(r) dV = 1 = \int_{S_{3}} \nabla G_{3}(r) \cdot \hat{\mathbf{n}} dS$$

$$\int_{S} \nabla^{2} G_{2}(r) dS = 1 = \oint_{C} \nabla G_{2}(r) \cdot \hat{\mathbf{n}} dl$$

where we have used the divergence theorem and its 2D analogue (usually called Green's theorem). Here S_3 is the surface of the sphere and C is the circumference of the circle. In both cases $\nabla G.\hat{\mathbf{n}} = \frac{dG}{dr}$ and we get

$$4\pi r^2 \frac{dG_3}{dr} = 1 \qquad 2\pi r \frac{G_2}{dr} = 1$$

and so

$$G_3(r) = -\frac{1}{4\pi r} + c_3 \tag{28}$$

$$G_2(r) = \frac{\log r}{2\pi} + c_2 \tag{29}$$

and $r = |\mathbf{r} - \mathbf{r}_0|$. In 3D we often apply the far field BC $G_3(r) \to 0$ as $r \to \infty$ setting $c_3 = 0$ to get the so-called **free-space Green's function**:

$$G_3(r) = -\frac{1}{4\pi |\mathbf{r} - \mathbf{r}_0|}.$$

Hereafter, G_3 will denote this function. In 2D we cannot apply an analogous far field condition. Note that these fundamental solutions satisfy the Laplace equation for all $\mathbf{r} \neq \mathbf{r}_0$ but at \mathbf{r}_0 they are *singular* so we need to exercise special care (cf. next section) in using them as Green's functions for the Poisson equation throughout a domain.

Green's identities

Green's identities (sometimes called Green's theorems, but not to be confused with the 2D version of the divergence theorem!) establish a relationship between the fundamental solutions G_2 and G_3 and solutions of Poisson's equation. We will discuss here only the 3D case. The 2D case is similar (exercise and cf. also exercise sheet IV).

For two scalar functions ϕ and ψ in some volume V with surface S and outward normal \hat{n} , the divergence theorem and product rule gives us that

$$\int_{V} \nabla \cdot (\phi \nabla \psi) \, dV = \int_{V} [\phi \nabla^{2} \psi + (\nabla \phi) \cdot (\nabla \psi)] \, dV = \int_{S} \phi \nabla \psi \cdot \hat{\mathbf{n}} \, dS,$$

which is **Green's first identity**. By simply interchanging the roles of ϕ and ψ we also have

$$\int_{S} \psi \nabla \phi . \hat{\mathbf{n}} \, dS = \int_{V} \left[\psi \nabla^{2} \phi + (\nabla \phi) . (\nabla \psi) \right] dV,$$

and subtracting this from the previous form we get Green's second identity:

$$\int_{S} \left(\phi \frac{\partial \psi}{\partial n} - \psi \frac{\partial \phi}{\partial n} \right) dS = \int_{V} \left[\phi \nabla^{2} \psi - \psi \nabla^{2} \phi \right] dV \tag{30}$$

(where we have written $\partial \phi / \partial n$ for $\nabla \phi . \hat{\mathbf{n}}$ etc.)

Now we'll want to use $\psi = G_3$ in Green's second identity but G_3 is singular at the point \mathbf{r}_0 in V so it is not a priori clear that eq. (30) will still hold (since the divergence theorem is usually stated as requiring functions that are regular throughout V). However below we will show that in fact, Green's second identity does hold with $\psi = G_3$. Then using $\nabla^2 G_3 = \delta(\mathbf{r} - \mathbf{r}_0)$ the first volume integral on RHS becomed $\phi(\mathbf{r}_0)$ and we obtain

$$\phi(\mathbf{r}_0) = \int_V G_3(\mathbf{r}; \mathbf{r}_0) \nabla^2 \phi \, dV + \int_S \left(\phi(\mathbf{r}) \frac{\partial G_3(\mathbf{r}; \mathbf{r}_0)}{\partial n} - G_3(\mathbf{r}; \mathbf{r}_0) \frac{\partial \phi(\mathbf{r})}{\partial n} \right) dS$$
(31)

(the integrations being over the space of variable \mathbf{r}).

To see that eq. (31) is actually valid, for simplicity let us choose the point \mathbf{r}_0 to be the origin. Then we define a new volume, V_{ϵ} , which is V with a little ball B_{ϵ} centred at the origin, of radius ϵ (and with surface S_{ϵ}), cut out of V. Now, in V_{ϵ} , G_3 is perfectly well-behaved, so we can legitimately apply Green's second identity in V_{ϵ} . Furthermore we have $\nabla^2 G_3 = 0$. Therefore eq. (30) gives

$$\int_{V_{\epsilon}} [\phi \nabla^{2} G_{3} - G_{3} \nabla^{2} \phi] dV = -\int_{V_{\epsilon}} G_{3} \nabla^{2} \phi dV$$

$$= \int_{S} \left(\phi \frac{\partial G_{3}}{\partial n} - G_{3} \frac{\partial \phi}{\partial n} \right) dS + \int_{S_{\epsilon}} \left(\phi \frac{\partial G_{3}}{\partial n} - G_{3} \frac{\partial \phi}{\partial n} \right) dS. \tag{32}$$

Now consider the behaviour of the surface integral over S_{ϵ} (second integral above), as ϵ becomes arbitrarily small. Since $G_3 = -1/(4\pi\epsilon)$ on S_{ϵ} the second term of the S_{ϵ} integral is

$$-\int_{S_{\epsilon}} G_3 \frac{\partial \phi}{\partial n} dS = \frac{1}{4\pi\epsilon} \int_{S_{\epsilon}} \frac{\partial \phi}{\partial n} dS = \frac{4\pi\epsilon^2}{4\pi\epsilon} \overline{A}_{\epsilon}$$

where \overline{A}_{ϵ} is the average value of $\frac{\partial \phi}{\partial n}$ on S_{ϵ} (i.e. the integral over the surface divided by the total surface area). Since ϕ is regular at the origin, $\overline{A}_{\epsilon} \to \frac{\partial \phi}{\partial n}|_{0}$ (a finite value) as $\epsilon \to 0$, and so the above integral tends to zero as $\epsilon \to 0$.

On the other hand, for the first term of the S_{ϵ} integral, the r derivative acts on $G_3 = -1/(4\pi r)$. Thus (remembering that the outward normal from V_{ϵ} on the surface S_{ϵ} points in the negative r direction) we get

$$\int_{S_{\epsilon}} \phi \frac{\partial G_3}{\partial n} \, dS = -\frac{1}{4\pi\epsilon^2} \int_{S_{\epsilon}} \phi \, dS = -\overline{\phi}$$

where $\overline{\phi}$ is the average value of ϕ over S_{ϵ} , which tends to $\phi(0)$ as $\epsilon \to 0$. Hence

$$\int_{S} \phi \frac{\partial G_3}{\partial n} dS \to -\phi(0) \quad \text{as} \quad \epsilon \to 0$$

Putting all this together, (and wlog removing the reliance on the special point \mathbf{r}_0 being at the origin) we get precisely eq. (31) as required.

Now returning to Poisson's equation $\nabla^2 \phi = -f$ we substitute $\phi = u$ into eq. (31) to get **Green's third identity**:

$$u(\mathbf{r}_{0}) = \int_{V} (-f(\mathbf{r}))G_{3}(\mathbf{r}; \mathbf{r}_{0}) dV + \int_{S} \left(u \frac{\partial G_{3}(\mathbf{r}; \mathbf{r}_{0})}{\partial n} - G_{3}(\mathbf{r}; \mathbf{r}_{0}) \frac{\partial u}{\partial n} \right) dS.$$
(33)

This is a remarkable formula, as it describes the solution throughout the interior of the domain in terms of the properties of the solution on the boundary (and the free-space Green's function) Also notice that (unlike the previous cases we have considered

in the course) the Green's function is here providing an expression for the solution with *in*homogeneous BCs.

Exercise: Green's third identity in 2D (cf. also exercise sheet IV).

Show that the equivalent result in two dimensions in a domain S with perimeter C (with arc length element dl) is

$$u(\mathbf{r}_0) = \int_S (-f)G_2 dS + \oint_C \left(u\frac{\partial G_2}{\partial n} - G_2\frac{\partial u}{\partial n}\right) dl,$$

where G_2 as defined by eq. (29) with $c_2 = 0$. \square

We make two remarks about eq. (33).

Remark. In the infinite domain of full 3D space, if u and $\frac{\partial u}{\partial n}$ tend to zero asymptotically suitably fast, then eq. (33) shows that G_3 is the free space Green's function for the Poisson equation. This also follows formally from $\nabla^2 G_3 = \delta(\mathbf{r} - \mathbf{r}_0)$, since if $u(\mathbf{r}_0) = \int_V -f(\mathbf{r})G_3(\mathbf{r} - \mathbf{r}_0) \, dV$ then (taking ∇^2 w.r.t. variable \mathbf{r}_0):

$$\nabla^2 u(\mathbf{r}_0) = \int_V -f(\mathbf{r})\nabla^2 G_3 dV = \int_V -f(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}_0) dV = -f(\mathbf{r}_0).$$

Remark. By setting f = 0, eq. (33) also provides an expression for the solution u of the Laplace equation in the interior of a domain, in terms of the values of u and $\frac{\partial u}{\partial n}$ on the boundary. But if \mathcal{D} is say, a closed bounded domain, then specification of u alone on the boundary already determines u (satisfying Laplace's equation) uniquely (the Dirichlet problem) and the normal derivative $\frac{\partial u}{\partial n}$ on the boundary cannot be freely independently specified. Similarly (Neumann problem) specifying $\frac{\partial u}{\partial n}$ on the boundary determines u up to an additive constant, so u cannot be freely specified on the boundary. Nevertheless eq. (33) is a valid expression for any function that is harmonic (i.e. a solution of the Laplace equation) in terms of its values of u and $\frac{\partial u}{\partial n}$ on the boundary. As such it is not a useful expression to solve for u in \mathcal{D} (since the surface data cannot be freely specified) but nevertheless it is a useful mathematical relation for proving further properties of harmonic functions.

In view of this curious "over-determined" property of eq. (33) we will now finally ask how can the Dirichlet problem, for the Laplace and Poisson equations, be solved using Green's function techniques, in domains with boundaries. One may also ask about the Neumann problem (where the normal derivative is specified on the boundary) but in this course we will discuss only the Dirichlet problem (in 3D here, and a 2D example is given on exercise sheet IV). One brief remark though, about the Neumann problem – it is somewhat more complicated than the Dirichlet problem since (unlike the Dirichlet case) a consistency condition must be satisfied by the boundary data if a solution is to exist at all. Indeed suppose $\frac{\partial u}{\partial n} = h(\mathbf{r})$ is specified on the boundary $\partial \mathcal{D}$. Then by the divergence theorem we must have

$$\int_{\partial \mathcal{D}} h \, dS = \int_{\partial \mathcal{D}} \nabla u \cdot n \, dS = \int_{\mathcal{D}} \nabla^2 u \, dV = -\int_{\mathcal{D}} f \, dV$$

(where f is the RHS forcing function in the Poisson equation) and this consistency condition then complicates the construction of a Green's function.

10.5 Dirichlet Green's functions

The **Dirichlet Green's function** for the Laplacian operator on some domain \mathcal{D} (containing both \mathbf{r} and \mathbf{r}_0) is defined be the function $G(\mathbf{r}; \mathbf{r}_0)$ such that:

(GR1): $G(\mathbf{r}; \mathbf{r}_0) = G_3(\mathbf{r}; \mathbf{r}_0) + H(\mathbf{r}, \mathbf{r}_0)$ where H is finite throughout \mathcal{D} (including at $\mathbf{r} = \mathbf{r}_0$) and H satisfies the Laplace equation throughout \mathcal{D} ; and

(GR2): $G(\mathbf{r}; \mathbf{r}_0) = 0$ on the boundary of \mathcal{D} i.e. G is G_3 modified by a harmonic function H chosen to make G zero on the boundary.

Note that G also satisfies the Laplace equation at all $\mathbf{r} \neq \mathbf{r}_0$.

Assuming for the moment that we can find such a Green's function, we are then able to find the solution to Poisson's equation on the domain \mathcal{D} with Dirichlet boundary conditions, as follows.

Let $\nabla^2 u = -f$ in \mathcal{D} with $u = h(\mathbf{r})$ given on $\partial \mathcal{D}$. Substituting $G_3 = G - H$ into Green's third identity eq. (33) gives

$$u(\mathbf{r}_0) = \int_{\partial \mathcal{D}} \left(u \frac{\partial (G - H)}{\partial n} - (G - H) \frac{\partial u}{\partial n} \right) dS + \int_{\mathcal{D}} (-f)(G - H) dV.$$
 (34)

Now H is harmonic throughout \mathcal{D} so Green's second identity (with u and H) gives

$$\int_{\partial \mathcal{D}} \left(u \frac{\partial H}{\partial n} - H \frac{\partial u}{\partial n} \right) dS = -\int_{\mathcal{D}} (-f) H dV.$$

Hence all the H terms in eq. (34) cancel and we get

$$u(\mathbf{r}_0) = \int_{\partial \mathcal{D}} \left(u(\mathbf{r}) \frac{\partial G(\mathbf{r}; \mathbf{r}_0)}{\partial n} - G(\mathbf{r}; \mathbf{r}_0) \frac{\partial u(\mathbf{r})}{\partial n} \right) dS + \int_{\mathcal{D}} [-f(\mathbf{r})] G(\mathbf{r}; \mathbf{r}_0) dV. \quad (35)$$

Finally having chosen H so that G is zero on $\partial \mathcal{D}$ (and $u = h(\mathbf{r})$ on $\partial \mathcal{D}$) we get

$$u(\mathbf{r}_0) = \int_{\partial \mathcal{D}} h(\mathbf{r}) \frac{\partial G(\mathbf{r}; \mathbf{r}_0)}{\partial n} dS + \int_{\mathcal{D}} [-f(\mathbf{r})] G(\mathbf{r}; \mathbf{r}_0) dV.$$
 (36)

This expression is now constructive, in the sense that the solution *throughout* the domain is given in terms of the known boundary conditions, and the Green's function.

Remark: if instead we had a Neumann problem with $\partial u/\partial n = k(\mathbf{r})$ being specified on the boundary $\partial \mathcal{D}$ then we would instead seek H in (GR1) to make $\partial G/\partial n = 0$ on $\partial \mathcal{D}$ in (GR2) (so H is defined up to an additive constant). Then from eq. (35) we get the solution to the Neumann problem as

$$u(\mathbf{r}_0) = \int_{\partial \mathcal{D}} -k(\mathbf{r})G(\mathbf{r}; \mathbf{r}_0) dS + \int_{\mathcal{D}} [-f(\mathbf{r})]G(\mathbf{r}; \mathbf{r}_0) dV.$$

Exercise: Symmetry of the Green's function

Using Green's second identity we can prove (cf. exercise sheet IV) that the Green's function is always symmetric, i.e. $G(\mathbf{r}; \mathbf{r}_0) = G(\mathbf{r}_0; \mathbf{r})$, for all $\mathbf{r} \neq \mathbf{r}_0$. This is the mathematical statement of the **principle of reciprocity** in electrostatics; a source at \mathbf{x} has the same effect at \mathbf{x}_0 as a source at \mathbf{x}_0 would have at \mathbf{x} .

10.6 Method of images

So how do we find the Green's function (G above, i.e a suitable H) in a domain with boundaries? In general this is difficult (i.e. we need to solve the Dirichlet problem for the Laplace equation with non-trivial BCs to get H!), but for domains with sufficient symmetry we can sometimes use the **method of images** (also called the reflection method) to construct the required Green's function. Indeed, this method can also be used for the Green's functions of the forced heat and wave equations too, as well as for homogeneous equations – the key concept is $match\ the\ boundary\ conditions$. We will illustrate it with some examples (cf. exercise sheet IV for more examples).

Example: Laplace equation – Dirichlet Green's function for the half-space

Consider a domain $\mathcal{D} = \{(x, y, z) : z > 0\}$. We want to find the solution to the following problem defined in \mathcal{D} :

$$\nabla^2 u = 0$$
, $u(\mathbf{x}) \to 0$ as $|\mathbf{x}| \to \infty$, $u(x, y, 0) = h(x, y)$.

To use the formula eq. (36), we need to construct a Green's function which satisfies the conditions (GR1) and (GR2), interpreting the zero boundary condition in the far field in the natural way of requiring $G \to 0$ as $|\mathbf{x}| \to \infty$. Since the problem has a natural Cartesian geometry, let us write $\mathbf{r} = \mathbf{x} = [x, y, z]$, and $\mathbf{r}_0 = \mathbf{x}_0^+ = [x_0, y_0, z_0]$.

We know that the free space Green's function G_3 satisfies all the conditions *except* the homogeneous BC G=0 boundary z=0. We need to "cancel" its nonzero values there while retaining all our other desired properties. To achieve this, the elegant **method of images** proceeds as follows:

Start from the free space Green's function and then try to add some other solution of Laplace's equation to it to get the required boundary condition. To do this, imagine that there is an **image** of the special point *outside* of the domain, exactly the same vertical distance away from the boundary as the special point i.e. we reflect the special point in the boundary as a mirror. To cancel the values of G_3 on the boundary we take the image as a point source with opposite sign, and postulate that

$$G(\mathbf{x}; \mathbf{x}_0) = \frac{-1}{4\pi |\mathbf{x} - \mathbf{x}_0^+|} + \frac{1}{4\pi |\mathbf{x} - \mathbf{x}_0^-|},$$

$$= -\frac{1}{4\pi} \left[(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2 \right]^{-1/2}$$

$$+ \frac{1}{4\pi} \left[(x - x_0)^2 + (y - y_0)^2 + (z + z_0)^2 \right]^{-1/2},$$

where $\mathbf{x}_0^- = [x_0, y_0, -z_0]$. Now since \mathbf{x}_0^- is definitely out of the domain, the second term satisfies Laplace's equation *everywhere* in \mathcal{D} , so we have (GR1). H and G_3 are both asymptotically zero at the far boundary $|\mathbf{x}| \to \infty$, and finally, for any point \mathbf{x}_b on the boundary z = 0, the two terms cancel perfectly; so we have (GR2). Therefore we have found the Dirichlet Green's function!

To apply the formula (36), note also that f = 0 (for Laplace's equation here) and also that there is no contribution from the far field since $u \to 0$ is the far field BC of the

problem. The *outward* normal from the domain at z = 0 is in the negative z-direction, and so the only contribution to the expression comes from the lower boundary, and is

$$\frac{\partial G}{\partial n}\Big|_{z=0} = -\frac{\partial G}{\partial z}\Big|_{z=0}
= \frac{1}{4\pi} \left(\frac{z+z_0}{|\mathbf{x}-\mathbf{x}_0^-|^3} - \frac{z-z_0}{|\mathbf{x}-\mathbf{x}_0^+|^3} \right)_{z=0}
= \frac{z_0}{2\pi} \left[(x-x_0)^2 + (y-y_0)^2 + z_0^2 \right]^{-3/2}.$$

Therefore we get

$$u(x_0, y_0, z_0) = \frac{z_0}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[(x - x_0)^2 + (y - y_0)^2 + z_0^2 \right]^{-3/2} h(x, y) \, dx \, dy,$$

as the solution of the Dirichlet problem for the Laplace equation in the half space.

The method of images can also be applied to some more complicated domains – e.g. for the domain $a \le z \le b$ between two planar boundaries, we can view the two boundaries as mirrors and then any special point \mathbf{r}_0 in the domain gives rise to a double infinity of multiply reflected images. If these are taken with alternating plus and minus signs, we can construct a Green's function that vanishes on both boundaries.

Example: Images for wave problems

We can also apply the method of images to the Green's functions that we developed for the forced wave and heat equations (with ICs all being zero). For example consider the semi-infinite domain $0 \le x < \infty$ and suppose we wish to impose the homogeneous Dirichlet condition $G(0,t;\xi,\tau)=0$ on the causal Green's function. Exactly the same idea applies as above: add an equal amplitude Green's function with opposite sign and having 'special point' not at ξ but at $-\xi$. For example, the appropriate Dirichlet Green's function for the wave equation is

$$G(x,t;\xi,\tau) = \frac{H(c[t-\tau] - |x-\xi|)}{2c} - \frac{H(c[t-\tau] - |x+\xi|)}{2c},$$

i.e. an odd function, which automatically imposes the zero Dirichlet boundary condition. Similarly for a homogeneous Neumann BC at x=0 viz.

$$\frac{\partial G(x,t;\xi,\tau)}{\partial x}\Big|_{x=0} = 0$$
 for all t ,

we make the derivative an odd function in x, which we achieve by an even extension of the Green's function. For example, the appropriate Neumann Green's function for the wave equation is

$$G(x,t;\xi,\tau) = \frac{H(c[t-\tau] - |x-\xi|)}{2c} + \frac{H(c[t-\tau] - |x+\xi|)}{2c},$$

and the image has the *same* sign. Indeed, for sufficiently small, yet still positive x, $|x - \xi| = \xi - x$, and $|x + \xi| = \xi + x$, so far all t

$$\frac{\partial G}{\partial x}\Big|_{x=0} = \frac{1}{2c} \left(\delta[c(t-\tau) - |x-\xi|][1] + \delta[c(t-\tau) - |x+\xi|][-1]\right)_{x=0}$$

$$= 0 \quad \text{for all } t$$

as desired.

Example: images for homogeneous problems

For homogeneous diffusion or wave equation problems we do not use a Green's function, but the method of images can still be applied to the initial data itself to adapt our previous solutions to be applicable in the presence of extra boundaries. For example consider the wave equation for y(x,t) on the half-line $x \geq 0$ with Neumann BC $y_x(0,t) = 0$ at the boundary x = 0, and with initial conditions

$$y(x,0) = b(x)$$
 $y_t(x,0) = 0$ for $x \ge 0$

where b(x) is the 'top-hat' function having value 1 in $[x_0 - a, x_0 + a]$ and zero elsewhere (and $a < x_0$) i.e. a box of width 2a, and height 1 centred on x_0 .

According to d'Alembert's general solution eq. (9), the solution for the whole line will be a pair of boxes, each of height half and width 2a, one going to the left and one going to the right, with speed c. This solution clearly does not satisfy the Neumann BC at x = 0 (when the left moving box passes over the origin). Thus we consider an initial image box (on the negative x axis) by reflecting the given ICs in x = 0 to extend the problem to the whole line (and take the image with a plus sign, for the Neumann condition).

Applying d'Alembert's solution we now have two pairs of moving boxes (of heights half). The solution satisfies the wave equation everywhere, satisfies the given ICs for $x \ge 0$ and satisfies the Neumann BC at x = 0 (as the solution is always an even function of x for any fixed t. Thus taking this solution restricted to just $x \ge 0$, we have solved our original problem!

It is instructive to picture how this solution evolves in time (especially in the region $x \geq 0$). Let B_R and B_L denote the right and left moving boxes for the original IC, and I_R and I_L the boxes from the image IC. I_L just moves off to the left and never appears as part of the solution for $x \geq 0$. B_R just moves off to the right and is always present in the $x \geq 0$ region. At time $t = (x_0 - a)/c$ both B_L and I_R reach x = 0 (with their respective leading edges). As they pass through each other (for a time 2a/c) the solution piles up to double height where they overlap and then B_L goes off into x < 0 while I_R emerges fully into $x \geq 0$. Thereafter, the solution in $x \geq 0$ is just two boxes of heights half, with centres separated by constant distance $2x_0$ (the initial separation of I_L and B_R) moving off to the right at speed c.

If we view the solution near x = 0 just on the positive side, we see B_L "hit the wall", piling up to double height (and enclosing the same total area at all times) as it appears to be reflected back to the right into x > 0 with final shape unchanged, giving the trailing second right-moving box.

The Neumann condition at x = 0 physically models small amplitude waves in the vicinity of a frictionless wall e.g. an elastic string for $x \ge 0$ (with zero gravity) that is attached to a vertical pole at x = 0 by a frictionless light (i.e. massless) ring, so the string can sustain no spatial gradient at x = 0 i.e. cannot have any vertical force component, and is thus always horizontal there.

$$====End\ of\ Notes!====$$