2.1 The Diffusion Equation

2.1.1 Introduction

The one-dimensional diffusion equation is the \textit{linear second order partial differential equation}

\[ u_t - Du_{xx} = f \]

where \( u = u(x, t) \), \( x \) is a real space variable, \( t \) a time variable and \( D \) a positive constant, called \textit{diffusion coefficient}. In space dimension \( n > 1 \), that is when \( x \in \mathbb{R}^n \), the diffusion equation reads

\[ u_t - D \Delta u = f \quad (2.1) \]

where \( \Delta \) denotes the \textit{Laplace operator}:

\[ \Delta = \sum_{k=1}^{n} \frac{\partial^2}{\partial x_k^2}. \]

When \( f \equiv 0 \) the equation is said to be \textit{homogeneous} and in this case the \textbf{superposition principle} holds: if \( u \) and \( v \) are solutions of (2.1) and \( a, b \) are real (or complex) numbers, \( au + bv \) also is a solution of (2.1). More generally, if \( u_k(x, t) \) is a family of solutions depending on the parameter \( k \) (integer or real) and \( g = g(k) \) is a function rapidly vanishing at infinity, then

\[ \sum_{k=1}^{\infty} u_k(x, t) g(k) \quad \text{and} \quad \int_{-\infty}^{+\infty} u_k(x, t) g(k) \, dk \]

are still solutions.
A common example of diffusion is given by heat conduction in a solid body. Conduction comes from molecular collision, transferring heat by kinetic energy, without macroscopic material movement. If the medium is homogeneous and isotropic with respect to the heat propagation, the evolution of the temperature is described by equation (2.1); $f$ represents the intensity of an external distributed source. For this reason equation (2.1) is also known as the heat equation.

On the other hand equation (2.1) constitutes a much more general diffusion model, where by diffusion we mean, for instance, the transport of a substance due to the molecular motion of the surrounding medium. In this case, $u$ could represent the concentration of a polluting material or of a solute in a liquid or a gas (dye in a liquid, smoke in the atmosphere) or even a probability density. We may say that the diffusion equation unifies at a macroscopic scale a variety of phenomena, that look quite different when observed at a microscopic scale.

Through equation (2.1) and some of its variants we will explore the deep connection between probabilistic and deterministic models, according (roughly) to the scheme

\[
\text{diffusion processes} \leftrightarrow \text{probability density} \leftrightarrow \text{differential equations}.
\]

The star in this field is Brownian motion, derived from the name of the botanist Brown, who observed in the middle of the 19th century, the apparently chaotic behavior of certain particles on a water surface, due to the molecular motion. This irregular motion is now modeled as a stochastic process under the terminology of Wiener process or Brownian motion. The operator

\[
\frac{1}{2} \Delta
\]

is strictly related to Brownian motion\(^1\) and indeed it captures and synthesizes the microscopic features of that process.

Under equilibrium conditions, that is when there is no time evolution, the solution $u$ depends only on the space variable and satisfies the stationary version of the diffusion equation (letting $D = 1$)

\[
-\Delta u = f
\]

($-u_{xx} = f$, in dimension $n = 1$). Equation (2.2) is known as the Poisson equation. When $f = 0$, it is called Laplace’s equation and its solutions are so important in so many fields that they have deserved the special name of harmonic functions. This equation will be considered in the next chapter.

### 2.1.2 The conduction of heat

Heat is a form of energy which it is frequently convenient to consider as separated from other forms. For historical reasons, calories instead of Joules are used as units of measurement, each calorie corresponding to 4.182 Joules.

\(^1\) In the theory of stochastic processes, $\frac{1}{2} \Delta$ represents the infinitesimal generator of the Brownian motion.
We want to derive a mathematical model for the heat conduction in a solid body. We assume that the body is homogeneous and isotropic, with constant mass density $\rho$, and that it can receive energy from an external source (for instance, from an electrical current or a chemical reaction or from external absorption/radiation). Denote by $r$ the time rate per unit mass at which heat is supplied\(^2\) by the external source.

Since heat is a form of energy, it is natural to use the law of conservation of energy, that we can formulate in the following way:

Let $V$ be an arbitrary control volume inside the body. The time rate of change of thermal energy in $V$ equals the net flux of heat through the boundary $\partial V$ of $V$, due to the conduction, plus the time rate at which heat is supplied by the external sources.

If we denote by $e = e(\mathbf{x}, t)$ the thermal energy per unit mass, the total quantity of thermal energy inside $V$ is given by

$$\int_V e \rho \, d\mathbf{x}$$

so that its time rate of change is\(^3\)

$$\frac{d}{dt} \int_V e \rho \, d\mathbf{x} = \int_V e_t \rho \, d\mathbf{x}.$$

Denote by $\mathbf{q}$ the heat flux vector\(^4\), which specifies the heat flow direction and the magnitude of the rate of flow across a unit area. More precisely, if $d\sigma$ is an area element contained in $\partial V$ with outer unit normal $\mathbf{v}$, then $\mathbf{q} \cdot \mathbf{v} d\sigma$ is the energy flow rate through $d\sigma$ and therefore the total inner heat flux through $\partial V$ is given by

$$- \int_{\partial V} \mathbf{q} \cdot \mathbf{v} \, d\sigma = \left(\text{divergence theorem}\right) - \int_V \text{div} \mathbf{q} \, d\mathbf{x}.$$

Finally, the contribution due to the external source is given by

$$\int_V r \rho \, d\mathbf{x}.$$

Thus, conservation of energy requires:

$$\int_V e_t \rho \, d\mathbf{x} = - \int_V \text{div} \mathbf{q} \, d\mathbf{x} + \int_V r \rho \, d\mathbf{x}. \quad (2.3)$$

The arbitrariness of $V$ allows us to convert the integral equation (2.3) into the pointwise relation

$$e_t \rho = - \text{div} \mathbf{q} + r \rho \quad (2.4)$$

\(^2\) Dimensions of $r$: $[r] = [\text{cal}] \times [\text{time}]^{-1} \times [\text{mass}]^{-1}$.

\(^3\) Assuming that the time derivative can be carried inside the integral.

\(^4\) $[\mathbf{q}] = [\text{cal}] \times [\text{length}]^{-2} \times [\text{time}]^{-1}$. 
that constitutes a basic law of heat conduction. However, \( e \) and \( q \) are unknown and we need additional information through constitutive relations for these quantities. We assume the following:

- **Fourier law** of heat conduction. Under “normal” conditions, for many solid materials, the heat flux is a linear function of the temperature gradient, that is:

\[
q = -\kappa \nabla u
\]  

(2.5)

where \( u \) is the absolute temperature and \( \kappa > 0 \), the thermal conductivity\(^5\), depends on the properties of the material. In general, \( \kappa \) may depend on \( u, x \) and \( t \), but often varies so little in cases of interest that it is reasonable to neglect its variation. Here we consider \( \kappa \) constant so that

\[
\text{div} q = -\kappa \Delta u.
\]  

(2.6)

The minus sign in the law (2.5) reflects the tendency of heat to flow from hotter to cooler regions.

- The thermal energy is a linear function of the absolute temperature:

\[
e = c_v u
\]  

(2.7)

where \( c_v \) denotes the specific heat\(^6\) (at constant volume) of the material. In many cases of interest \( c_v \) can be considered constant. The relation (2.7) is reasonably true over not too wide ranges of temperature.

Using (2.6) and (2.7), equation (2.4) becomes

\[
u_t = \frac{\kappa}{c_v \rho} \Delta u + \frac{1}{c_v} f
\]  

(2.8)

which is the diffusion equation with \( D = \kappa / (c_v \rho) \) and \( f = r / c_v \). As we will see, the coefficient \( D \), called thermal diffusivity, encodes the thermal response time of the material.

### 2.1.3 Well posed problems \((n = 1)\)

As we have mentioned at the end of chapter one, the governing equations in a mathematical model have to be supplemented by additional information in order to obtain a well posed problem, i.e. a problem that has exactly one solution, depending continuously on the data.

On physical grounds, it is not difficult to outline some typical well posed problems for the heat equation. Consider the evolution of the temperature \( u \) inside a cylindrical bar, whose lateral surface is perfectly insulated and whose length is much larger than its cross-sectional area \( A \). Although the bar is three dimensional,

---

\(^5\) \([\kappa] = [\text{cal}] \times [\text{deg}]^{-1} \times [\text{time}]^{-1} \times [\text{length}]^{-1} \) (deg stays for degree, Celsius or Kelvin).

\(^6\) \([c_v] = [\text{cal}] \times [\text{deg}]^{-1} \times [\text{mass}]^{-1} \).
we may assume that heat moves only down the length of the bar and that the heat transfer intensity is uniformly distributed in each section of the bar. Thus we may assume that $e = e(x,t)$, $r = r(x,t)$, with $0 \leq x \leq L$. Accordingly, the constitutive relations (2.5) and (2.7) read
\[
e(x,t) = c_v u(x,t), \quad q = -\kappa u_x i.
\]
By choosing $V = A \times [x, x + \Delta x]$ as the control volume in (2.3), the cross-sectional area $A$ cancels out, and we obtain
\[
\int_x^{x+\Delta x} c_v \rho u_t \, dx = \int_x^{x+\Delta x} \kappa u_{xx} \, dx + \int_x^{x+\Delta x} r \rho \, dx
\]
that yields for $u$ the one-dimensional heat equation
\[
u_t - Du_{xx} = f.
\]
We want to study the temperature evolution during an interval of time, say, from $t = 0$ until $t = T$. It is then reasonable to prescribe its initial distribution inside the bar: different initial configurations will correspond to different evolutions of the temperature along the bar. Thus we need to prescribe the initial condition
\[
u(x,0) = g(x)
\]
where $g$ models the initial temperature profile.
This is not enough to determine a unique evolution; it is necessary to know how the bar interacts with the surroundings. Indeed, starting with a given initial temperature distribution, we can change the evolution of $u$ by controlling the temperature or the heat flux at the two ends of the bar\footnote{Remember that the bar has perfect lateral thermal insulation.}; for instance, we could keep the temperature at a certain fixed level or let it vary in a certain way, depending on time. This amounts to prescribing
\[
u(0,t) = h_1(t), \quad u(L,t) = h_2(t)
\]
(2.9) at any time $t \in (0,T]$. The (2.9) are called Dirichlet boundary conditions.
We could also prescribe the heat flux at the end points. Since from Fourier law we have
\[
\text{inward heat flow at } x = 0 : -\kappa u_x (0,t)
\]
\[
\text{inward heat flow at } x = L : \kappa u_x (L,t)
\]
the heat flux is assigned through the Neumann boundary conditions
\[
-u_x (0,t) = h_1(t), \quad u_x (L,t) = h_2(t)
\]
at any time $t \in (0,T]$.\footnote{Remember that the bar has perfect lateral thermal insulation.}
Another type of boundary condition is the **Robin** or radiation condition. Let the surroundings be kept at temperature \( U \) and assume that the inward heat flux from one end of the bar, say \( x = L \), depends linearly on the difference \( U - u \), that is\(^8\)

\[
\kappa u_x = \gamma (U - u) \quad (\gamma > 0).
\]

(2.10)

Letting \( \alpha = \gamma / \kappa > 0 \) and \( h = \gamma U / \kappa \), the Robin condition at \( x = L \) reads

\[
u_x + \alpha u = h.\]

Clearly, it is possible to assign **mixed conditions**: for instance, at one end a Dirichlet condition and at the other one a Neumann condition.

The problems associated with the above boundary conditions have a corresponding nomenclature. Summarizing, we can state the most common problems for the one dimensional heat equation as follows: given \( f = f(x,t) \) (external source) and \( g = g(x) \) (initial or Cauchy data), determine \( u = u(x,t) \) such that:

\[
\begin{cases}
\quad u_t - Du_{xx} = f \quad &0 < x < L, 0 < t < T \\
\quad u(x,0) = g(x) \quad &0 \leq x \leq L \\
\quad + \text{boundary conditions} \quad &0 < t \leq T
\end{cases}
\]

where the boundary conditions may be:

- **Dirichlet**:
  \[
  u(0,t) = h_1(t), \quad u(L,t) = h_2(t),
  \]

- **Neumann**:
  \[
  -u_x(0,t) = h_1(t), \quad u_x(L,t) = h_2(t),
  \]

- **Robin or radiation**:
  \[
  -u_x(0,t) + \alpha u(0,t) = h_1(t), \quad u_x(L,t) + \alpha u(L,t) = h_2(t) \quad (\alpha > 0),
  \]

or **mixed** conditions. Accordingly, we have the initial-Dirichlet problem, the initial-Neumann problem and so on. When \( h_1 = h_2 = 0 \), we say that the boundary conditions are **homogeneous**.

**Remark 2.1.** Observe that only a special part of the boundary of the rectangle

\[
Q_T = (0,L) \times (0,T),
\]

called the parabolic boundary of \( Q_T \), carries the data (see Fig. 2.1). No final condition (for \( t = T, 0 < x < L \)) is required.

\(^8\) Formula (2.10) is based on Newton's law of cooling: the heat loss from the surface of a body is a linear function of the temperature drop \( U - u \) from the surroundings to the surface. It represents a good approximation to the radiative loss from a body when \(|U - u|/u \ll 1\).
Fig. 2.1. The parabolic boundary of $Q_T$

In important applications, for instance in financial mathematics, $x$ varies over unbounded intervals, typically $(0, \infty)$ or $\mathbb{R}$. In these cases one has to require that the solution do not grow too much at infinity. We will later consider the global Cauchy problem:

\[
\begin{aligned}
&u_t - Du_{xx} = f & \quad x \in \mathbb{R}, 0 < t < T \\
&u(x, 0) = g(x) & \quad x \in \mathbb{R} \\
&+ \text{ conditions as } x \to \pm \infty.
\end{aligned}
\]

2.1.4 A solution by separation of variables

We will prove that under reasonable hypotheses the initial Dirichlet, Neumann or Robin problems are well posed. Sometimes this can be shown using elementary techniques like the separation of variables method that we describe below through a simple example of heat conduction. We will come back to this method from a more general point of view in Section 6.9.

As in the previous section, consider a bar (that we can consider one-dimensional) of length $L$, initially (at time $t = 0$) at constant temperature $u_0$. Thereafter, the end point $x = 0$ is kept at the same temperature while the other end $x = L$ is kept at a constant temperature $u_1 > u_0$. We want to know how the temperature evolves inside the bar.

Before making any computations, let us try to conjecture what could happen. Given that $u_1 > u_0$, heat starts flowing from the hotter end, raising the temperature inside the bar and causing a heat outflow into the cold boundary. On the other hand, the interior increase of temperature causes the hot inflow to decrease in time, while the outflow increases. We expect that sooner or later the two fluxes balance each other and that the temperature eventually reaches a steady state.
distribution. It would also be interesting to know how fast the steady state is reached.

We show that this is exactly the behavior predicted by our mathematical model, given by the heat equation

\[ u_t - Du_{xx} = 0 \quad t > 0, 0 < x < L \]

with the initial-Dirichlet conditions

\[
\begin{align*}
  u (x, 0) & = g (x) & 0 \leq x \leq L \\
  u (0, t) & = u_0, u (L, t) = u_1 & t > 0.
\end{align*}
\]

Since we are interested in the long term behavior of our solution, we leave \( t \) unlimited. Notice the \textit{jump discontinuity} between the initial and the boundary data at \( x = L \); we will take care of this little difficulty later.

- \textbf{Dimensionless variables.} First of all we introduce dimensionless variables, that is variables \textit{independent of the units of measurement}. To do that we rescale space, time and temperature with respect to quantities that are characteristic of our problem. For the space variable we can use the length \( L \) of the bar as rescaling factor, setting

\[
y = \frac{x}{L}
\]

which is clearly dimensionless, being a ratio of lengths. Notice that

\[
0 \leq y \leq 1.
\]

How can we rescale time? Observe that the dimensions of the diffusion coefficient \( D \) are

\[
[length]^2 \times [time]^{-1}.
\]

Thus the constant \( \tau = L^2 / D \) gives a characteristic time scale for our diffusion problem. Therefore we introduce the dimensionless time

\[
s = \frac{t}{\tau}, \tag{2.11}
\]

Finally, we rescale the temperature by setting

\[
z (y, s) = \frac{u (Ly, \tau s) - u_0}{u_1 - u_0}.
\]

For the dimensionless temperature \( z \) we have:

\[
\begin{align*}
  z (y, 0) & = \frac{u (Ly, 0) - u_0}{u_1 - u_0} = 0, & 0 \leq y \leq 1 \\
  z (0, s) & = \frac{u (0, \tau s) - u_0}{u_1 - u_0} = 0, & z (1, s) = \frac{u (L, \tau s) - u_0}{u_1 - u_0} = 1.
\end{align*}
\]
Moreover
\[
(u_1 - u_0) z_s = \frac{\partial t}{\partial s} u_t = \tau u_t = \frac{L^2}{D} u_t
\]
\[
(u_1 - u_0) z_{yy} = \left( \frac{\partial x}{\partial y} \right)^2 u_{xx} = L^2 u_{xx}.
\]
Hence, since \( u_t = Du_{xx} \),
\[
(u_1 - u_0)(z_s - z_{yy}) = \frac{L^2}{D} u_t - L^2 u_{xx} = \frac{L^2}{D} Du_{xx} - L^2 u_{xx} = 0.
\]
In conclusion, we find
\[
z_s - z_{yy} = 0 \quad (2.12)
\]
with the initial condition
\[
z (y, 0) = 0 \quad (2.13)
\]
and the boundary conditions
\[
z (0, s) = 0, \quad z (1, s) = 1. \quad (2.14)
\]
We see that in the dimensionless formulation the parameters \( L \) and \( D \) have disappeared, emphasizing the mathematical essence of the problem. On the other hand, we will show later the relevance of the dimensionless variables in test modelling.

- **The steady state solution.** We start solving problem (2.12), (2.13), (2.14) by first determining the steady state solution \( z_{st} \), that satisfies the equation \( z_{yy} = 0 \) and the boundary conditions (2.14). An elementary computation gives
\[
z_{st} (y) = y.
\]
In terms of the original variables the steady state solution is
\[
u_{st} (x) = u_0 + (u_1 - u_0) \frac{x}{L}
\]
corresponding to a uniform heat flux along the bar given by the Fourier law:
\[
\text{heat flux} = -\kappa u_x = -\kappa \frac{(u_1 - u_0)}{L}.
\]
- **The transient regime.** Knowing the steady state solution, it is convenient to introduce the function
\[
U (y, s) = z_{st} (y, s) - z (y, s) = y - z (y, s).
\]
Since we expect our solution to eventually reach the steady state, \( U \) represents a transient regime that should converge to zero as \( s \to \infty \). Furthermore, the rate of convergence to zero of \( U \) gives information on how fast the temperature reaches its equilibrium distribution. \( U \) satisfies (2.12) with initial condition
\[
U (y, 0) = y \quad (2.15)
\]
and *homogeneous* boundary conditions

\[
U(0, s) = 0 \quad \text{and} \quad U(1, s) = 0. \tag{2.16}
\]

- *The method of separation of variables.* We are now in a position to find an explicit formula for \( U \) using the method of separation of variables. The main idea is to exploit the linear nature of the problem constructing the solution by superposition of simpler solutions of the form \( w(s)v(y) \) in which the variables \( s \) and \( y \) appear in *separated form.*

**Step 1.** We look for non-trivial solutions of (2.12) of the form

\[
U(y, s) = w(s)v(y)
\]

with \( v(0) = v(1) = 0 \). By substitution in (2.12) we find

\[
0 = U_s - U_{yy} = w'(s)v(y) - w(s)v''(y)
\]

from which, separating the variables,

\[
\frac{w'(s)}{w(s)} = \frac{v''(y)}{v(y)}. \tag{2.17}
\]

Now, the left hand side in (2.17) is a function of \( s \) only, while the right hand side is a function of \( y \) only and the equality must hold for every \( s > 0 \) and every \( y \in (0, L) \). This is possible only when both sides are equal to a common constant \( \lambda \), say. Hence we have

\[
v''(y) - \lambda v(y) = 0 \tag{2.18}
\]

with

\[
v(0) = v(1) = 0 \tag{2.19}
\]

and

\[
w'(s) - \lambda w(s) = 0. \tag{2.20}
\]

**Step 2.** We first solve problem (2.18), (2.19). There are three different possibilities for the general solution of (2.18):

a) If \( \lambda = 0 \),

\[
v(y) = A + By \quad (A, B \text{ arbitrary constants})
\]

and the conditions (2.19) imply \( A = B = 0 \).

b) If \( \lambda \) is a positive real number, say \( \lambda = \mu^2 > 0 \), then

\[
v(y) = Ae^{-\mu y} + Be^{\mu y}
\]

and again it is easy to check that the conditions (2.19) imply \( A = B = 0 \).

c) Finally, if \( \lambda = -\mu^2 < 0 \), then

\[
v(y) = A \sin \mu y + B \cos \mu y.
\]
From (2.19) we get
\[ v(0) = B = 0 \]
\[ v(1) = A \sin \mu + B \cos \mu = 0 \]
from which
\[ A \text{ arbitrary, } B = 0, \mu_m = m\pi, \ m = 1, 2, \ldots . \]
Thus, only in case c) we find non-trivial solutions
\[ v_m(y) = A \sin m\pi y. \quad (2.21) \]
In this context, (2.18), (2.19) is called an eigenvalue problem; the special values \( \mu_m \) are the eigenvalues and the solutions \( v_m \) are the corresponding eigenfunctions. With \( \lambda = -\mu_m^2 = -m^2\pi^2 \), the general solution of (2.20) is
\[ w_m(s) = Ce^{-m^2\pi^2 s} \quad (C \text{ arbitrary constant}). \quad (2.22) \]
From (2.21) and (2.22) we obtain damped sinusoidal waves of the form
\[ U_m(y, s) = A_m e^{-m^2\pi^2 s} \sin m\pi y. \]

Step 3. Although the solutions \( U_m \) satisfy the homogeneous Dirichlet conditions, they do not match, in general, the initial condition \( U(y, 0) = y \). As we already mentioned, we try to construct the correct solution superposing the \( U_m \) by setting
\[ U(y, s) = \sum_{m=1}^{\infty} A_m e^{-m^2\pi^2 s} \sin m\pi y. \quad (2.23) \]
Some questions arise:

Q1. The initial condition requires
\[ U(y, 0) = \sum_{m=1}^{\infty} A_m \sin m\pi y = y \quad \text{for } 0 \leq y \leq 1. \quad (2.24) \]
Is it possible to choose the coefficients \( A_m \) in order to satisfy (2.24)? In which sense does \( U \) attain the initial data? For instance, is it true that
\[ U(z, s) \to y \quad \text{if} \quad (z, s) \to (y, 0)? \]

Q2. Any finite linear combination of the \( U_m \) is a solution of the heat equation; can we make sure that the same is true for \( U \)? The answer is positive if we could differentiate term by term the infinite sum and get
\[ (\partial_s - \partial_{yy}^2)U(y, s) = \sum_{m=1}^{\infty} (\partial_s - \partial_{yy})U_m(y, s) = 0. \quad (2.25) \]
What about the boundary conditions?

Q3. Even if we have a positive answer to questions 1 and 2, are we confident that \( U \) is the unique solution of our problem and therefore that it describes the correct evolution of the temperature?

Q1. Question 1 is rather general and concerns the Fourier series expansion\(^9\) of a function, in particular of the initial data \( f(y) = y \), in the interval \((0,1)\). Due to the homogeneous Dirichlet conditions it is convenient to expand \( f(y) = y \) in a sine Fourier series, whose coefficients are given by the formulas

\[
A_m = 2 \int_0^1 y \sin m\pi y \, dy = -\frac{2}{m\pi} [y \cos m\pi y]_0^1 + \frac{2}{m\pi} \int_0^1 \cos m\pi y \, dy = -2 \frac{\cos m\pi}{m\pi} = (-1)^{m+1} \frac{2}{m\pi}.
\]

The sine Fourier expansion of \( f(y) = y \) is therefore

\[
y = \sum_{m=1}^{\infty} (-1)^{m+1} \frac{2}{m\pi} \sin m\pi y.
\]

(2.26)

Where is the expansion (2.26) valid? It cannot be true at \( y = 1 \) since \( \sin m\pi = 0 \) for every \( m \) and we would obtain \( 1 = 0 \). This clearly reflects the jump discontinuity of the data at \( y = 1 \).

The theory of Fourier series implies that (2.26) is true at every point \( y \in [0,1) \) and that the series converges uniformly in every interval \([0,a], a < 1\). Moreover, equality (2.26) holds in the least square sense (or \( L^2(0,1) \) sense), that is

\[
\int_0^1 [y - \sum_{m=1}^{N} (-1)^{m+1} \frac{2}{m\pi} \sin m\pi y]^2 \, dy \to 0 \quad \text{as } N \to \infty.
\]

From (2.23) and the expression of \( A_m \), we obtain the formal solution

\[
U(y,s) = \sum_{m=1}^{\infty} (-1)^{m+1} \frac{2}{m\pi} e^{-m^2\pi^2 s} \sin m\pi y
\]

(2.27)

that attains the initial data in the least squares sense, i.e.\(^10\).

\[
\lim_{s \to 0^+} \int_0^1 [U(y,s) - y]^2 \, dy = 0.
\]

(2.28)

In fact, from Parseval’s equality\(^11\), we can write

\[
\int_0^1 [U(y,s) - y]^2 \, dy = \frac{4}{\pi^2} \sum_{m=1}^{\infty} \left( e^{-m^2\pi^2 s} - 1 \right)^2.
\]

(2.29)

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\(9\) Appendix A.

\(10\) It is also true that \( U(z,s) \to y \) in the pointwise sense, when \( y \neq 1 \) and \( (z,s) \to (y,0) \).

\(11\) We omit the proof.

Appendix A.
Since for \( s \geq 0 \)
\[
\frac{\left(e^{-m^2\pi^2s} - 1\right)^2}{m^2} \leq \frac{1}{m^2}
\]
and the series \( \sum 1/m^2 \) converges, then the series (2.29) converges uniformly by the Weierstrass test (see Section 1.4) in \([0, \infty)\) and we can take the limit under the sum, obtaining (2.28).

Q2. The analytical expression of \( U \) is rather reassuring: it is a superposition of sinusoids of increasing frequency \( m \) and of strongly damped amplitude because of the negative exponential, at least when \( s > 0 \). Indeed, for \( s > 0 \), the rapid convergence to zero of each term and its derivatives in the series (2.27) allows us to differentiate term by term. Precisely, we have
\[
\frac{\partial U_m}{\partial s} = (-1)^{m+2} 2m\pi e^{-m^2\pi^2s} \sin m\pi y, \quad \frac{\partial^2 U_m}{\partial y^2} = (-1)^{m+2} 2e^{-m^2\pi^2s} \sin m\pi y
\]
so that, if \( s \geq s_0 > 0 \),
\[
\left| \frac{\partial U_m}{\partial s} \right| \leq 2m\pi e^{-m^2\pi^2s_0}, \quad \left| \frac{\partial^2 U_m}{\partial y^2} \right| \leq 2m\pi e^{-m^2\pi^2s_0}.
\]
Since the numerical series
\[
\sum_{m=1}^{\infty} me^{-m^2\pi^2s_0}
\]
is convergent, we conclude by the Weierstrass test that the series
\[
\sum_{m=1}^{\infty} \frac{\partial U_m}{\partial s} \quad \text{and} \quad \sum_{m=1}^{\infty} \frac{\partial^2 U_m}{\partial y^2}
\]
converge uniformly in \([0, 1] \times [s_0, \infty)\) so that (2.25) is true and therefore \( U \) is a solution of (2.12).

It remains to check the Dirichlet conditions: if \( s_0 > 0 \),
\[
U(z, s) \to 0 \quad \text{as} \quad (z, s) \to (0, s_0) \quad \text{or} \quad (z, s) \to (L, s_0).
\]
This is true because we can take the two limits under the sum, due to the uniform convergence of the series (2.27) in any region \([0, L] \times (b, +\infty)\) with \( b > 0 \). For the same reason, \( U \) has continuous derivatives of any order, up to the lateral boundary of the strip \([0, L] \times (b, +\infty)\).

Note, in particular, that \( U \) immediately forgets the initial discontinuity and becomes smooth at any positive time.

Q3. To show that \( U \) is indeed the unique solution, we use the so-called energy method, that we will develop later in greater generality. Suppose \( W \) is another solution of problem (2.12), (2.15), (2.16). Then, by linearity,
\[
v = U - W
\]
satisfies
\[ v_s - v_{yy} = 0 \] (2.30)
and has zero initial-boundary data. Multiplying (2.30) by \( v \), integrating in \( y \) over the interval \([0, 1]\) and keeping \( s > 0 \), fixed, we get
\[ \int_0^1 vv_s \, dy - \int_0^1 vv_{yy} \, dy = 0. \] (2.31)
Observe that
\[ \int_0^1 vv_s \, dy = \frac{1}{2} \int_0^1 \partial_y (v^2) \, dy = \frac{1}{2} \frac{d}{ds} \int_0^1 v^2 \, dy. \] (2.32)
Moreover, integrating by parts we can write
\[ \int_0^1 vv_{yy} \, dy = [v(1, s) v_y(1, s) - v(0, s) v_y(0, s)] - \int_0^1 (v_y)^2 \, dy \] (2.33)
\[ = - \int_0^1 (v_y)^2 \, dy \]
since \( v(1, s) = v(0, s) = 0 \). From (2.31), (2.32) and (2.33) we get
\[ \frac{1}{2} \frac{d}{ds} \int_0^1 v^2 \, dy = - \int_0^1 (v_y)^2 \, dy \leq 0 \] (2.34)
and therefore, the nonnegative function
\[ E(s) = \int_0^1 v^2(y, s) \, dy \]
is non-increasing. On the other hand, using (2.28) for \( v \) instead of \( U \), we get
\[ E(s) \to 0 \quad \text{as} \quad s \to 0 \]
which forces \( E(s) = 0 \), for every \( s > 0 \). But \( v^2(y, s) \) is nonnegative and continuous in \([0, 1]\) if \( s > 0 \), so that it must be \( v(y, s) = 0 \) for every \( s > 0 \) or, equivalently, \( U = W \).

- **Back to the original variables.** In terms of the original variables, our solution is expressed as
\[ u(x, t) = u_0 + (u_1 - u_0) \frac{x}{L} - \sum_{m=1}^{\infty} (-1)^{m+1} \frac{2}{m \pi} e^{-m^2 \pi^2 D L^2 t} \sin \frac{m \pi}{L} x. \]
This formula confirms our initial guess about the evolution of the temperature towards the steady state. Indeed, each term of the series converges to zero exponentially as \( t \to +\infty \) and it is not difficult to show\(^{12}\) that
\[ u(x, t) \to u_0 + (u_1 - u_0) \frac{x}{L} \quad \text{as} \quad t \to +\infty. \]
\(^{12}\) The Weierstrass test works here for \( t \geq t_0 > 0 \).
Moreover, among the various terms of the series, the first one \( m = 1 \) decays much more slowly than the others and very soon it determines the main deviation of \( u \) from the equilibrium, *independently of the initial condition*. This leading term is the damped sinusoid

\[
\frac{2}{\pi} e^{-\pi^2 D t} \sin \frac{\pi}{L} x.
\]

In this mode there is a concentration of heat at \( x = L/2 \) where the temperature reaches its maximum amplitude \( 2 \exp(-\pi^2 D t/L^2)/\pi \). At time \( t = L^2/D \) the amplitude decays to \( 2 \exp(-\pi^2)/\pi \simeq 3.3 \times 10^{-5} \), about 0.005 per cent of its initial value. This simple calculation shows that to reach the steady state a time of order \( L^2/D \) is required, a fundamental fact in heat diffusion.

Not surprisingly, the scaling factor in (2.11) was exactly \( \tau = L^2/D \). The dimensionless formulation is extremely useful in experimental modelling tests. To achieve reliable results, these models must reproduce the same characteristics at different scales. For instance, if our bar were an experimental model of a much bigger beam of length \( L_0 \) and diffusion coefficient \( D_0 \), to reproduce the same heat diffusion effects, we must choose material \((D)\) and length \((L)\) for our model bar such that

\[
\frac{L^2}{D} = \frac{L_0^2}{D_0}.
\]

Figure 2.2 shows the solution of the dimensionless problem (2.12), (2.15), (2.16) for \( 0 < t \leq 1 \).

\[\text{Fig. 2.2. The solution to the dimensionless problem (2.12), (2.13), (2.14)}\]

### 2.1.5 Problems in dimension \( n > 1 \)

The formulation of the well posed problems in subsection 2.1.3 can be easily generalized to any spatial dimension \( n > 1 \), in particular to \( n = 2 \) or \( n = 3 \). Suppose we want to determine the evolution of the temperature in a heat conducting body that occupies a bounded domain\(^{13}\) \( \Omega \subset \mathbb{R}^n \), during an interval of time \([0, T]\). Under the hypotheses of subsection 2.1.2, the temperature is a function \( u = u(x,t) \)

\(^{13}\) Recall that by *domain* we mean an *open connected set* in \( \mathbb{R}^n \).
that satisfies the heat equation $u_t - D \Delta u = f$, in the space-time cylinder

$$Q_T = \Omega \times (0, T).$$

To select a unique solution we have to prescribe first of all the initial distribution

$$u(x, 0) = g(x) \quad x \in \Omega,$$

where $\overline{\Omega} = \Omega \cup \partial \Omega$ denotes the closure of $\Omega$.

The control of the interaction of the body with the surroundings is modeled through suitable conditions on $\partial \Omega$. The most common ones are:

**Dirichlet condition**: the temperature is kept at a prescribed level on $\partial \Omega$; this amounts to assigning

$$u(\sigma, t) = h(\sigma, t) \quad \sigma \in \partial \Omega \text{ and } t \in (0, T].$$

**Neumann condition**: the heat flux through $\partial \Omega$ is assigned. To model this condition, we assume that the boundary $\partial \Omega$ is a smooth curve or surface, having a tangent line or plane at every point\(^{14}\) with outward unit vector $\nu$. From Fourier law we have

$$q = \text{heat flux} = -\kappa \nabla u$$

so that the inward heat flux is

$$-q \cdot \nu = \kappa \nabla u \cdot \nu = \kappa \partial_\nu u.$$

Thus the Neumann condition reads

$$\partial_\nu u(\sigma, t) = h(\sigma, t) \quad \sigma \in \partial \Omega \text{ and } t \in (0, T].$$

**Radiation or Robin condition**: the inward (say) heat flux through $\partial \Omega$ depends linearly on the difference\(^{15}\) $U - u$:

$$-q \cdot \nu = \gamma (U - u) \quad (\gamma > 0)$$

where $U$ is the ambient temperature. From the Fourier law we obtain

$$\partial_\nu u + \alpha u = h \quad \text{on } \partial \Omega \times (0, T]$$

with $\alpha = \gamma / \kappa > 0$, $h = \gamma U / \kappa$.

**Mixed conditions**: the boundary of $\Omega$ is decomposed into various parts where different boundary conditions are prescribed. For instance, a formulation of a mixed Dirichlet-Neumann problem is obtained by writing

$$\partial \Omega = \partial D \Omega \cup \partial N \Omega \quad \text{with} \quad \partial D \Omega \cap \partial N \Omega = \emptyset$$

\(^{14}\) We can also allow boundaries with corner points, like squares, cones, or edges, like cubes. It is enough that the set of points where the tangent plane does not exist has zero surface measure (zero length in two dimensions). Lipschitz domains have this property (see Section 1.4).

\(^{15}\) Linear Newton law of cooling.
where \( \partial_D \Omega \) and \( \partial_N \Omega \) “reasonable” subsets of \( \partial \Omega \). Typically \( \partial_N \Omega = \partial \Omega \cap A \), where \( A \) is open in \( \mathbb{R}^n \). In this case we say that \( \partial_N \Omega \) is a relatively open set in \( \partial \Omega \). Then we assign

\[
\begin{align*}
  u &= h_1 \text{ on } \partial_D \Omega \times (0, T] \\
  \partial_N u &= h_2 \text{ on } \partial_N \Omega \times (0, T].
\end{align*}
\]

Summarizing, we have the following typical problems: given \( f = f(\mathbf{x}, t) \) and \( g = g(\mathbf{x}) \), determine \( u = u(\mathbf{x}, t) \) such that:

\[
\begin{align*}
  \left\{ \begin{array}{l}
    u_t - D \Delta u = f & \text{in } Q_T \\
    u(\mathbf{x}, 0) = g(\mathbf{x}) & \text{in } \overline{\Omega}
  \end{array} \right.
\]

+ boundary conditions on \( \partial \Omega \times (0, T] \)

where the boundary conditions are:

- **Dirichlet:**
  \[
  u = h,
  \]

- **Neumann:**
  \[
  \partial_N u = h,
  \]

- **radiation or Robin:**
  \[
  \partial_N u + \alpha u = h \quad (\alpha > 0),
  \]

- **mixed:**
  \[
  u = h_1 \text{ on } \partial_D \Omega, \quad \partial_N u = h_2 \text{ on } \partial_N \Omega.
  \]

![Fig. 2.3. The space-time cylinder \( Q_T \)](image)

Also in dimension \( n > 1 \), the *global Cauchy problem* is important:

\[
\begin{align*}
  \left\{ \begin{array}{l}
    u_t - D \Delta u = f & \mathbf{x} \in \mathbb{R}^n, \ 0 < t < T \\
    u(\mathbf{x}, 0) = g(\mathbf{x}) & \mathbf{x} \in \mathbb{R}^n
  \end{array} \right.
\]

+ condition as \( |\mathbf{x}| \to \infty \).
Remark 2.2. We again emphasize that no final condition (for \( t = T, x \in \Omega \)) is required. The data is assigned on the parabolic boundary \( \partial_p Q_T \) of \( Q_T \), given by the union of the bottom points \( \bar{\Omega} \times \{ t = 0 \} \) and the side points \( \partial \Omega \times (0, T] \):

\[
\partial_p Q_T = (\bar{\Omega} \times \{ t = 0 \}) \cup (\partial \Omega \times (0, T]).
\]

2.2 Uniqueness

2.2.1 Integral method

Generalizing the energy method used in subsection 2.1.4, it is easy to show that all the problems we have formulated in the previous section have at most one solution under reasonable conditions on the data. Suppose \( u \) and \( v \) are solutions of one of those problems, sharing the same boundary conditions, and let \( w = u - v \); we want to show that \( w \equiv 0 \). For the time being we do not worry about the precise hypotheses on \( u \) and \( v \); we assume they are sufficiently smooth in \( Q_T \) up to \( \partial_p Q_T \) and observe that \( w \) satisfies the homogeneous equation

\[
w_t - D \Delta w = 0 \tag{2.35}
\]

in \( Q_T = \Omega \times (0, T) \), with initial condition

\[w(x, 0) = 0\]

in \( \bar{\Omega} \), and one of the following conditions on \( \partial \Omega \times (0, T] \):

\[w = 0 \quad \text{(Dirichlet)} \tag{2.36}
\]

or

\[
\partial_\nu w = 0 \quad \text{(Neumann)} \tag{2.37}
\]

or

\[
\partial_\nu w + \alpha w = 0 \quad \alpha > 0, \quad \text{(Robin)} \tag{2.38}
\]

or

\[w = 0 \text{ on } \partial D \Omega, \quad \partial_\nu w = 0 \text{ on } \partial N \Omega \quad \text{(mixed)}. \tag{2.39}\]

Multiply equation (2.35) by \( w \) and integrate on \( \Omega \); we find

\[
\int_\Omega w w_t \, dx = D \int_\Omega w \Delta w \, dx.
\]

Now,

\[
\int_\Omega w w_t \, dx = \frac{1}{2} \frac{d}{dt} \int_\Omega w^2 \, dx \tag{2.40}
\]

and from Green’s identity (1.13) with \( u = v = w \),

\[
\int_\Omega w \Delta w \, dx = \int_{\partial \Omega} w \partial_\nu w \, d\sigma - \int_\Omega |\nabla w|^2 \, dx. \tag{2.41}
\]
Then, letting
\[ E(t) = \int_{\Omega} w^2 \, dx, \]
(2.40) and (2.41) give
\[ \frac{1}{2} E'(t) = D \int_{\partial \Omega} w \partial_{\nu} w \, d\sigma - D \int_{\Omega} |\nabla w|^2 \, dx. \]
If Robin condition (2.38) holds,
\[ \int_{\partial \Omega} w \partial_{\nu} w \, d\sigma = -\alpha \int_{\Omega} w^2 \, dx \leq 0. \]
If one of the (2.36), (2.37), (2.39) holds, then
\[ \int_{\partial \Omega} w \partial_{\nu} w \, d\sigma = 0. \]
In any case it follows that
\[ E'(t) \leq 0 \]
and therefore \( E \) is a nonincreasing function. Since
\[ E(0) = \int_{\Omega} w^2(x,0) \, dx = 0, \]
we must have \( E(t) = 0 \) for every \( t \geq 0 \) and this implies \( w(x,t) \equiv 0 \) in \( \Omega \) for every \( t > 0 \). Thus \( u = v \).

The above calculations are completely justified if \( \Omega \) is a sufficiently smooth domain\(^{16}\) and, for instance, we require that \( u \) and \( v \) are continuous in \( \overline{Q}_T = \overline{\Omega} \times [0,T] \), together with their first and second spatial derivatives and their first order time derivatives. We denote the set of these functions by the symbol (not too appealing...)
\[ C^{2,1}(\overline{Q}_T) \]
and synthesize everything in the following statement.

**Theorem 2.1.** The initial Dirichlet, Neumann, Robin and mixed problems have at most one solution belonging to \( C^{2,1}(\overline{Q}_T) \).

### 2.2.2 Maximum principles

The fact that heat flows from higher to lower temperature regions implies that a solution of the homogeneous heat equation attains its maximum and minimum values on \( \partial_p Q_T \). This result is known as the *maximum principle*. Moreover the equation reflects the time irreversibility of the phenomena that it describes, in the
\(^{16}\) \( C^1 \) or even Lipschitz domains, for instance (see Section 1.4).
sense that the future cannot have an influence on the past (causality principle). In other words, the value of a solution $u$ at time $t$ is independent of any change of the data after $t$.

The following simple theorem translates these principles and holds for functions in the class $C^{2,1}(Q_T) \cap C(\overline{Q_T})$. These functions are continuous up to the boundary of $Q_T$, with derivatives continuous in the interior of $Q_T$.

**Theorem 2.2.** Let $w \in C^{2,1}(Q_T) \cap C(\overline{Q_T})$ such that

$$w_t - D\Delta w = q \leq 0 \quad \text{in } Q_T. \quad (2.42)$$

Then $w$ attains its maximum on $\partial_p Q_T$:

$$\max_{\overline{Q_T}} w = \max_{\partial_p Q_T} w. \quad (2.43)$$

In particular, if $w$ is negative on $\partial_p Q_T$, then is negative in all $Q_T$.

**Proof.** We split the proof into two steps.

1. Let $\varepsilon > 0$ such that $T - \varepsilon > 0$. We prove that

$$\max_{\overline{Q_{T-\varepsilon}}} w \leq \max_{\partial_p Q_{T-\varepsilon}} w + \varepsilon T. \quad (2.44)$$

Let $u = w - \varepsilon t$. Then

$$u_t - D\Delta u = q - \varepsilon < 0. \quad (2.45)$$

We claim that the maximum of $u$ on $\overline{Q_{T-\varepsilon}}$ occurs on $\partial_p Q_{T-\varepsilon}$. Suppose not. Let $(x_0, t_0)$, $x_0 \in \Omega$, $0 < t_0 \leq T - \varepsilon$ be a maximum point for $u$ on $\overline{Q_{T-\varepsilon}}$. From elementary calculus, we have

$$\Delta u(x_0, t_0) \leq 0$$

and either

$$u_t(x_0, t_0) = 0 \quad \text{if } t_0 < T - \varepsilon$$

or

$$u_t(x_0, T - \varepsilon) \geq 0.$$

In both cases

$$u_t(x_0, t_0) - \Delta u(x_0, t_0) \geq 0,$$

contradicting (2.45). Thus

$$\max_{\overline{Q_{T-\varepsilon}}} u \leq \max_{\partial_p Q_{T-\varepsilon}} u \leq \max_{\partial_p Q_T} w \quad (2.46)$$

since $u \leq w$. On the other hand, $w \leq u + \varepsilon T$, and therefore, from (2.46) we get

$$\max_{\overline{Q_{T-\varepsilon}}} w \leq \max_{\overline{Q_{T-\varepsilon}}} w + \varepsilon T \leq \max_{\partial_p Q_T} w + \varepsilon T$$

which is (2.44).
Step 2. Since $w$ is continuous in $\overline{Q}_T$, we deduce that (why?)

$$\max_{\overline{Q}_{T-\varepsilon}} w \rightarrow \max_{\overline{Q}_T} w \quad \text{as} \quad \varepsilon \rightarrow 0.$$ 

Hence, letting $\varepsilon \rightarrow 0$ in (2.44) we find $\max_{\overline{Q}_T} w \leq \max_{\partial_p Q_T} w$ which concludes the proof. □

As an immediate consequence of Theorem 2.2 (see Problem 2.4) we have that if

$$w_t - D\Delta w = 0 \quad \text{in} \quad Q_T$$

then $w$ attains its maximum and its minimum on $\partial_p Q_T$. In particular

$$\min_{\partial_p Q_T} w \leq w(x,t) \leq \max_{\partial_p Q_T} w \quad \text{for every} \quad (x,t) \in Q_T.$$ 

Moreover:

**Corollary 2.1. (Comparison and stability).** Let $v$ and $w$ satisfy

$$v_t - D\Delta v = f_1 \quad \text{and} \quad w_t - D\Delta w = f_2.$$ 

Then:

a) If $v \geq w$ on $\partial_p Q_T$ and $f_1 \geq f_2$ in $Q_T$ then $v \geq w$ in all $Q_T$.

b) The following stability estimate holds

$$\max_{Q_T} |v - w| \leq \max_{\partial_p Q_T} |v - w| + T \max_{Q_T} |f_1 - f_2|. \quad (2.47)$$

In particular the initial-Dirichlet problem has at most one solution that, moreover, depends continuously on the data.

For the proof see Problem 2.5.

**Remark 2.3.** Corollary 2.1 gives uniqueness for the initial-Dirichlet problem under much less restrictive hypotheses than Theorem 2.1: indeed it does not require the continuity of any derivatives of the solution up to $\partial_p Q_T$.

Inequality (2.47) is a uniform pointwise stability estimate, extremely useful in several applications. In fact if $v = g_1$, $w = g_2$ on $\partial_p Q_T$ and

$$\max_{\partial_p Q_T} |g_1 - g_2| \leq \varepsilon \quad \text{and} \quad \max_{Q_T} |f_1 - f_2| \leq \varepsilon,$$

we deduce

$$\max_{Q_T} |v - w| \leq \varepsilon (1 + T).$$

Thus, in finite time, a small uniform distance between the data implies small uniform distance between the corresponding solutions.
Remark 2.4. **Strong maximum principle.** Theorem 2.2 is a version of the so called weak maximum principle, weak because this result says nothing about the possibility that a solution achieves its maximum or minimum at an interior point as well. Actually a more precise result is known as strong maximum principle and states\textsuperscript{17} that if a solution of \( u_t - D\Delta u = 0 \) achieves its maximum \( M \) (minimum) at a point \( (x_1, t_1) \) with \( x_1 \in V, \ 0 < t_1 \leq T \), then \( u = M \) in \( \bar{V} \times [0, t_1] \).

\[ u(x_1, t_1) = M = \max_{\partial V} u \]

Fig. 2.4. The strong maximum principle

2.3 The Fundamental Solution

There are privileged solutions of the diffusion equation that can be used to construct many other solutions. In this section we are going to discover one of these special building blocks, the most important one.

2.3.1 Invariant transformations

The \textit{homogeneous} diffusion equation has simple but important properties. Let \( u = u(x, t) \) be a solution of

\[ u_t - D\Delta u = 0. \tag{2.48} \]

- **Time reversal.** The function

\[ v(x, t) = u(x, -t), \]

obtained by the change of variable \( t \mapsto -t \), is a solution of the \textbf{adjoint} or \textbf{backward} equation.

\[ v_t + D\Delta v = 0. \]

\textsuperscript{17} We omit the rather long proof.
2.3 The Fundamental Solution

Coherently, the (2.48) is sometimes called the **forward** equation. The non-invariance of (2.48) with respect to a change of sign in time is another aspect of time irreversibility.

- **Space and time translations invariance.** For \(y, s\) fixed, the function
  \[ v(x,t) = u(x - y, t - s), \]
is still a solution of (2.48). Clearly, for \(x, t\) fixed the function \(u(x - y, t - s)\) is a solution of the **backward** equation with respect to \(y\) and \(s\).

- **Parabolic dilations** The transformation
  \[ x \mapsto ax, \quad t \mapsto bt, \quad u \mapsto cu \quad (a, b, c > 0) \]
represents a dilation (or contraction) of the graph of \(u\). Let us check for which values of \(a, b, c\) the function
  \[ u^* (x,t) = cu(ax, bt) \]
is still a solution of (2.48). We have:
  \[ u_t^* (x,t) - D\Delta u^* (x,t) = cbu_t (ax, bt) - ca^2 D\Delta u (ax, bt) \]
and so \(u^*\) is a solution of (2.48) if
  \[ b = a^2. \quad (2.49) \]
The relation (2.49) suggests the name of **parabolic dilation** for the transformation
  \[ x \mapsto ax \quad t \mapsto a^2 t \quad (a, b > 0). \]
Under this transformation the expressions
  \[ \frac{|x|^2}{Dt} \quad \text{or} \quad \frac{x}{\sqrt{Dt}} \]
are left unchanged. Moreover, we already observed that they are **dimensionless groups**. Thus it is not surprising that these combinations of the independent variables occur frequently in the study of diffusion phenomena.

- **Dilations and conservation of mass (or energy).** Let \(u = u(x, t)\) be a solution of (2.48) in the half-space \(\mathbb{R}^n \times (0, +\infty)\). Then we just checked that the function
  \[ u^* (x,t) = cu (ax, a^2 t) \quad (a > 0) \]
is also a solution in the same set. Suppose \(u\) satisfies the condition
  \[ \int_{\mathbb{R}^n} u(x, t) \, dx = q \quad \text{for every } t > 0. \quad (2.50) \]
If, for instance, $u$ represents the concentration of a substance (density of mass), equation (2.50) states that the total mass is $q$ at every time $t$. If $u$ is a temperature, (2.50) says that the total internal energy is constant ($= qpc_v$). We ask for which $a, c$ the solution $u^*$ still satisfies (2.50). We have

$$\int_{\mathbb{R}^n} u^*(x, t) \, dx = c \int_{\mathbb{R}^n} u(ax, a^2t) \, dx.$$ 

Letting $y = ax$, so that $dy = a^n \, dx$, we find

$$\int_{\mathbb{R}^n} u^*(x, t) \, dx = ca^{-n} \int_{\mathbb{R}^n} u(y, a^2t) \, dy = ca^{-n}$$

and for (2.50) to be satisfied we must have:

$$c = qa^n.$$ 

In conclusion, if $u = u(x, t)$ is a solution of (2.48) in the half-space $\mathbb{R}^n \times (0, +\infty)$ satisfying (2.50), the same is true for

$$u^*(x, t) = qa^n u(ax, a^2t).$$

(2.51)

### 2.3.2 Fundamental solution ($n = 1$)

We are now in position to construct our special solution, starting with dimension $n = 1$. To help intuition, think for instance of our solution as the concentration of a substance of total mass $q$ and suppose we want to keep the total mass equal to $q$ at any time.

We have seen that the combination of variables $x/\sqrt{Dt}$ is not only invariant with respect to parabolic dilations but also dimensionless. It is then natural to check if there are solutions of (2.48) involving such dimensionless group. Since $\sqrt{Dt}$ has the dimension of a length, the quantity $q/\sqrt{Dt}$ is a typical order of magnitude for the concentration, so that it makes sense to look for solutions of the form

$$u^*(x, t) = \frac{q}{\sqrt{Dt}} U \left( \frac{x}{\sqrt{Dt}} \right)$$

(2.52)

where $U$ is a (dimensionless) function of a single variable.

Here is the main question: is it possible to determine $U = U(\xi)$ such that $u^*$ is a solution of (2.48)? Solutions of the form (2.52) are called *similarity solutions*.\(^\text{18}\)

\(^\text{18}\) A solution of a particular evolution problem is a *similarity* or *self-similar* solution if its spatial configuration (graph) remains similar to itself at all times during the evolution. In one space dimension, *self-similar* solutions have the general form

$$u(x, t) = a(t) F(x/b(t))$$

where, preferably, $u/a$ and $x/b$ are dimensionless quantity.
Moreover, since we are interpreting \( u^* \) as a concentration, we require \( U \geq 0 \) and the total mass condition yields

\[
1 = \frac{1}{\sqrt{Dt}} \int_{\mathbb{R}} U \left( \frac{x}{\sqrt{Dt}} \right) dx = \frac{1}{\sqrt{Dt}} \int_{\mathbb{R}} U (\xi) d\xi
\]

so that we require that

\[
\int_{\mathbb{R}} U (\xi) d\xi = 1. \tag{2.53}
\]

Let us check if \( u^* \) is a solution to (2.48). We have

\[
u_t^* = \frac{q}{\sqrt{D}} \left[ -\frac{1}{2} t^{-\frac{3}{2}} U (\xi) - \frac{1}{2} t^{-2} U' (\xi) \right]
\]

\[
= -\frac{q}{2t\sqrt{Dt}} [U (\xi) + \xi U' (\xi)]
\]

\[
u_{xx}^* = \frac{q}{(Dt)^{3/2}} U'' (\xi),
\]

hence

\[
u_t^* - Du_{xx}^* = -\frac{q}{t\sqrt{Dt}} \left\{ U'' (\xi) + \frac{1}{2} \xi U' (\xi) + \frac{1}{2} U (\xi) \right\}.
\]

We see that for \( u^* \) to be a solution of (2.48), \( U \) must be a solution in \( \mathbb{R} \) of the ordinary differential equation

\[
U'' (\xi) + \frac{1}{2} \xi U' (\xi) + \frac{1}{2} U (\xi) = 0. \tag{2.54}
\]

Since \( U \geq 0 \), (2.53) implies\(^{19}\):

\[
U (-\infty) = U (+\infty) = 0.
\]

On the other hand, (2.54) is invariant with respect to the change of variables

\[
\xi \mapsto -\xi
\]

and therefore we look for even solutions: \( U (-\xi) = U (\xi) \). Then we can restrict ourselves to \( \xi \geq 0 \), asking

\[
U' (0) = 0 \text{ and } U (+\infty) = 0. \tag{2.55}
\]

\(^{19}\) Rigorously, the precise conditions are:

\[
\liminf_{x \to \pm \infty} U (x) = 0.
\]
To solve (2.54) observe that it can be written in the form
\[
\frac{d}{d\xi} \left\{ U'(\xi) + \frac{1}{2} \xi U(\xi) \right\} = 0
\]
that yields
\[
U'(\xi) + \frac{1}{2} \xi U(\xi) = C \quad (C \in \mathbb{R}). \tag{2.56}
\]
Letting \( \xi = 0 \) in (2.56) and recalling (2.55) we deduce that \( C = 0 \) and therefore
\[
U'(\xi) + \frac{1}{2} \xi U(\xi) = 0. \tag{2.57}
\]
The general integral of (2.57) is
\[
U(\xi) = c_0 e^{-\xi^2/4} \quad (c_0 \in \mathbb{R}).
\]
This function is even, positive, integrable and vanishes at infinity. It only remains to choose \( c_0 \) in order to ensure (2.53). Since\(^{20}\)
\[
\int_{\mathbb{R}} e^{-\xi^2/4} d\xi = 2 \int_{\mathbb{R}} e^{-z^2} dz = 2\sqrt{\pi}
\]
the choice is \( c_0 = (4\pi)^{-1/2} \).

Going back to the original variables, we have found the following solution of (2.48)
\[
u^*(x,t) = \frac{q}{\sqrt{4\pi Dt}} e^{-x^2/4Dt}, \quad x \in \mathbb{R}, t > 0
\]
positive, even in \( x \), and such that
\[
\int_{\mathbb{R}} u^*(x,t) dx = q \quad \text{for every } t > 0. \tag{2.58}
\]
The choice \( q = 1 \) gives a family of Gaussians, parametrized with time, and it is natural to think of a normal probability density.

\textbf{Definition 2.1.} The function
\[
\Gamma_D(x,t) = \frac{1}{\sqrt{4\pi Dt}} e^{-x^2/4Dt}, \quad x \in \mathbb{R}, t > 0
\]
is called the \textit{fundamental solution} of equation (2.48).

\(^{20}\) Recall that
\[
\int_{\mathbb{R}} e^{-z^2} = \sqrt{\pi}.
\]
2.3 The Fundamental Solution

2.3.3 The Dirac distribution

It is worthwhile to examine the behavior of the fundamental solution. For every fixed $x \neq 0$,

$$\lim_{t \to 0^+} \Gamma_D(x, t) = \lim_{t \to 0^+} \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}} = 0$$  \hspace{1cm} (2.60)

while

$$\lim_{t \to 0^+} \Gamma_D(0, t) = \lim_{t \to 0^+} \frac{1}{\sqrt{4\pi Dt}} = +\infty.$$  \hspace{1cm} (2.61)

If we interpret $\Gamma_D$ as a probability density, equations (2.60), (2.61) and (2.58) imply that when $t \to 0^+$ the fundamental solution tends to concentrate mass around the origin; eventually, the whole probability mass is concentrated at $x = 0$ (see Fig. 2.5).

The limiting density distribution can be mathematically modeled by the so-called Dirac distribution (or measure) at the origin, denoted by the symbol $\delta_0$ or simply by $\delta$. The Dirac distribution is not a function in the usual sense of Analysis; if it were, it should have the following properties:

- $\delta(0) = \infty$, $\delta(x) = 0$ for $x \neq 0$
- $\int_{\mathbb{R}} \delta(x) \, dx = 1$,

which are clearly incompatible with any concept of classical function or integral. A rigorous definition of the Dirac measure requires the theory of generalized functions or distributions of L. Schwartz, that we will consider in Chapter 7. Here we restrict ourselves to some heuristic considerations.

Let

$$\mathcal{H}(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0, \end{cases}$$

Fig. 2.5. The fundamental solution $\Gamma_1$ for $-4 < x < 4$, $0 < t < 1$
be the characteristic function of the interval \([0, \infty)\), known as the Heaviside function. Observe that

\[
\frac{\mathcal{H}(x + \varepsilon) - \mathcal{H}(x - \varepsilon)}{2\varepsilon} = \begin{cases} 
\frac{1}{2\varepsilon} & \text{if } -\varepsilon \leq x < \varepsilon \\
0 & \text{otherwise.}
\end{cases} \tag{2.62}
\]

Denote by \(I_\varepsilon(x)\) the quotient (2.62); the following properties hold:

i) For every \(\varepsilon > 0\),

\[
\int_{\mathbb{R}} I_\varepsilon(x) \, dx = \frac{1}{2\varepsilon} \times 2\varepsilon = 1.
\]

We can interpret \(I_\varepsilon\) as a unit impulse of extent \(2\varepsilon\) (Fig. 2.6).

ii) \[
\lim_{\varepsilon \downarrow 0} I_\varepsilon(x) = \begin{cases} 
0 & \text{if } x \neq 0 \\
\infty & \text{if } x = 0.
\end{cases}
\]

iii) If \(\varphi = \varphi(x)\) is a smooth function, vanishing outside a bounded interval, (a test function), we have

\[
\int_{\mathbb{R}} I_\varepsilon(x) \varphi(x) \, dx = \frac{1}{2\varepsilon} \int_{-\varepsilon}^{\varepsilon} \varphi(x) \, dx \xrightarrow{\varepsilon \to 0} \varphi(0). 
\]

Properties i) e ii) say that \(I_\varepsilon\) tends to a mathematical object that has precisely the formal features of the Dirac distribution at the origin. In particular iii) suggests how to identify this object, that is through its action on test functions.

**Definition 2.2.** We call Dirac measure at the origin the generalized function, denoted by \(\delta\), that acts on a test function \(\varphi\) as follows:

\[
\delta[\varphi] = \varphi(0). \tag{2.63}
\]

Equation (2.63) is often written in the form \(\langle \delta, \varphi \rangle = \varphi(0)\) or even

\[
\int \delta(x) \varphi(x) \, dx = \varphi(0)
\]
where the integral symbol is purely formal. Observe that property ii) shows that
\[ H' = \delta \]
whose meaning is given in the following computations, where an integration by parts is used and \( \varphi \) is a test function:
\[ \int_{\mathbb{R}} \varphi dH = - \int_{\mathbb{R}} H \varphi' = - \int_{0}^{\infty} \varphi' = \varphi(0), \tag{2.64} \]
\[ \text{since } \varphi \text{ vanishes for large} \]
\[ \text{With the notion of Dirac measure at hand, we can say that } \Gamma_D \text{ satisfies the initial conditions} \]
\[ \Gamma_D(x, 0) = \delta. \]
If the unit mass is concentrated at a point \( y \neq 0 \), we denote by \( \delta_y \) or \( \delta(x - y) \) the Dirac measure at \( y \), defined through the formula
\[ \int \delta(x - y) \varphi(x) \, dx = \varphi(y). \]
Then, by translation invariance, the fundamental solution \( \Gamma_D(x - y, t) \) is a solution of the diffusion equation, that satisfies the initial condition
\[ \Gamma_D(x - y, 0) = \delta(x - y). \]
Indeed it is the unique solution satisfying the total mass condition (2.58) with \( q = 1 \).

As any solution \( u \) of (2.48) has several interpretations (concentration of a substance, probability density, temperature in a bar) so the fundamental solution can have several meanings.

We can think of it as a \textbf{unit source solution}: \( \Gamma_D(x, t) \) gives the concentration at the point \( x \) at time \( t \), generated by the diffusion of a \textbf{unit mass initially} (\( t = 0 \)) \textbf{concentrated at the origin}. From another point of view, if we imagine a unit mass composed of a large number \( N \) of particles, \( \Gamma_D(x, t) \, dx \) gives the probability that a single particle is placed between \( x \) and \( x + dx \) at time \( t \) or equivalently, the percentage of particles inside the interval \((x, x + dx)\) at time \( t \).

Initially \( \Gamma_D \) is zero outside the origin. As soon as \( t > 0 \), \( \Gamma_D \) becomes positive everywhere: this amounts to saying that the unit mass diffuses instantaneously all over the \( x \)–axis and therefore with \textit{infinite speed of propagation}. This could be a problem in using (2.48) as a realistic model, although (see Fig. 2.5) for \( t > 0 \), small, \( \Gamma_D \) is practically zero outside an interval centered at the origin of length \( 4D \).

\[ \text{The first integral in (2.64) is a Riemann-Stieltjes integral, that formally can be written as} \]
\[ \int \varphi(x) \mathcal{H}'(x) \, dx \]
\[ \text{and interpreted as } \text{the action of the generalized function } \mathcal{H}' \text{ on the test function } \varphi. \]
2.3.4 Fundamental solution \((n > 1)\)

In space dimension greater than 1, we can more or less repeat the same arguments. We look for positive, radial, self-similar solutions \(u^*\) to (2.48), with total mass equal to \(q\) at every time, that is

\[
\int_{\mathbb{R}^n} u^*(x, t) \, dx = q \quad \text{for every } t > 0. \tag{2.65}
\]

Since \(q/(Dt)^{n/2}\) is a concentration per unit volume, we set

\[
u^*(x, t) = \frac{q}{(Dt)^{n/2}} U(\xi), \quad \xi = |x|/\sqrt{Dt}.
\]

We have, recalling the expression of the Laplace operator for radial functions (see Appendix C),

\[
u_t^* = -\frac{1}{2t(Dt)^{n/2}} \left[ nU(\xi) + \xi U'(\xi) \right]
\]

\[
\Delta u^* = \frac{1}{(Dt)^{1+n/2}} \left\{ U''(\xi) + \frac{n-1}{\xi} U'(\xi) \right\}.
\]

Therefore, for \(u^*\) to be a solution of (2.48), \(U\) must be a nonnegative solution in \((0, +\infty)\) of the ordinary differential equation

\[
\xi U''(\xi) + (n - 1) U'(\xi) + \frac{\xi^2}{2} U'(\xi) + \frac{n}{2} \xi U(\xi) = 0. \tag{2.66}
\]

Multiplying by \(\xi^{n-2}\), we can write (2.66) in the form

\[
(\xi^{n-1}U')' + \frac{1}{2} (\xi^n U)' = 0
\]

that gives

\[
\xi^{n-1}U' + \frac{1}{2} \xi^n U = C \quad (C \in \mathbb{R}). \tag{2.67}
\]

Assuming that \(\lim_{\xi \to 0^+}\) of \(U\) and \(U'\) are finite, letting \(\xi \to 0^+\) into (2.67), we deduce \(C = 0\) and therefore

\[
U' + \frac{1}{2} \xi U = 0.
\]

Thus we obtain the family of solutions

\[
U(\xi) = \frac{c_0}{2} e^{-\xi^2/4}.
\]

The total mass condition requires

\[
1 = \frac{1}{(Dt)^{n/2}} \int_{\mathbb{R}^n} U \left( \frac{|x|}{\sqrt{Dt}} \right) \, dx = \frac{c_0}{(Dt)^{n/2}} \int_{\mathbb{R}^n} \exp \left( -\frac{|x|^2}{4Dt} \right) \, dx
\]
2.4 Symmetric Random Walk ($n = 1$)

\[
y = x / \sqrt{D t} \quad c_0 \int_{\mathbb{R}^n} e^{-|y|^2} \, dy = c_0 \left( \int_{\mathbb{R}} e^{-z^2} \, dz \right)^n = c_0 \left( 4\pi \right)^{n/2}
\]

and therefore $c_0 = (4\pi)^{-n/2}$. Thus, we have obtained solutions of the form

\[
u^*(x, t) = \frac{q}{(4\pi Dt)^{n/2}} \exp \left( -\frac{|x|^2}{4Dt} \right), \quad (t > 0).
\]

Once more, the choice $q = 1$ is special.

**Definition 2.3.** The function

\[
\Gamma_D (x, t) = \frac{1}{(4\pi Dt)^{n/2}} \exp \left( -\frac{|x|^2}{4Dt} \right) \quad (t > 0)
\]

is called the **fundamental solution** of the diffusion equation (2.48).

The remarks after Definition 2.2 can be easily generalized to the multidimensional case. In particular, it is possible to define the $n-$ dimensional Dirac measure at a point $y$ through the formula\(^{22}\)

\[
\int \delta (x - y) \varphi (x) \, dx = \varphi (y) \quad (2.68)
\]

that expresses the action on the test function $\varphi$, smooth in $\mathbb{R}^n$ and vanishing outside a compact set. For fixed $y$, the fundamental solution $\Gamma_D (x - y, t)$ is the unique solution of the global Cauchy problem

\[
\begin{cases}
u_t - D \Delta u = 0 & x \in \mathbb{R}^n, t > 0 \\
u (x, 0) = \delta (x - y) & x \in \mathbb{R}^n
\end{cases}
\]

that satisfies (2.65) with $q = 1$.

## 2.4 Symmetric Random Walk ($n = 1$)

In this section we start exploring the connection between probabilistic and deterministic models, in dimension $n = 1$. The main purpose is to construct a Brownian motion, which is a **continuous model** (in both space and time), as a limit of a simple stochastic process, called random walk, which is instead a **discrete model** (in both space and time). During the realization of the limiting procedure we shall see how the diffusion equation can be approximated by a difference equation. Moreover, this new perspective will better clarify the nature of the diffusion coefficient.

\(^{22}\) As in dimension $n = 1$, in (2.68) the integral has a symbolic meaning only.
2.4.1 Preliminary computations

Consider a unit mass particle that moves randomly along the $x$ axis, according to the following rules: fix

\begin{align*}
\cdot & h > 0, \text{ space step} \\
\cdot & \tau > 0, \text{ time step}.
\end{align*}

1. During an interval of time $\tau$, the particle takes one step of $h$ unit length, starting from $x = 0$.
2. The particle moves to the left or to the right with probability $p = \frac{1}{2}$, independently of the previous step (Fig. 2.7).

At time $t = N\tau$, after $N$ steps, the particle will be at a point $x = mh$, where $N \geq 0$ and $m$ are integers, $-N \leq m \leq N$.

Our task is: Compute the probability $p(x,t)$ of finding the particle at $x$ at time $t$.

![Fig. 2.7. Symmetric random walk](image)

Random walks can be found in a wide variety of situations. To give an example, think of a gambling game in which a fair coin is thrown. If heads comes out, the particle moves to the right and the player gains 1 dollar; if tails comes out it moves to the left and the player loses 1 dollar: $p(x,t)$ is the probability to gain $m$ dollars after $N$ throws.

- **Computation of $p(x,t)$**.

Let $x = mh$ be the position of the particle after $N$ steps. To reach $x$, the particle takes some number of steps to the right, say $k$, and $N - k$ steps to the left. Clearly, $0 \leq k \leq N$ and

$$m = k - (N - k) = 2k - N$$

so that $N$ and $m$ are both even or both odd integers and

$$k = \frac{1}{2} (N + m).$$

Thus, $p(x,t) = p_k$ where

$$p_k = \frac{\text{number of walks with } k \text{ steps to the right after } N \text{ steps}}{\text{number of possible walks after } N \text{ steps}}. \quad (2.70)$$

---

$23$ One can also think of a large number of particles of total mass one.
Now, the number of possible walks with \( k \) steps to the right and \( N - k \) to the left is given by the binomial coefficient\(^{24}\)

\[
C_{N,k} = \binom{N}{k} = \frac{N!}{k!(N-k)!}.
\]

On the other hand, the number of possible walks after \( N \) steps is \( 2^N \) (why?); hence, from (2.70):

\[
p_k = \frac{C_{N,k}}{2^N} \quad x = mh, \quad t = N\tau, \quad k = \frac{1}{2} (N + m).
\]

- **Mean displacement and standard deviation of** \( x \).

Our ultimate goal is to let \( h \) and \( \tau \) go to zero in order to get a continuous walk, which incorporates the main features of the discrete random walk. This is a delicate point, since, if we want to obtain eventually a continuous faithful copy of the random walk, we need to isolate some quantitative parameters able to capture the essential features of the walk and maintain them unchanged. In our case there are two key parameters\(^{25}\):

(a) the **mean displacement** of \( x \) after \( N \) steps = \( \langle x \rangle = \langle m \rangle h \)

(b) the **second moment** of \( x \) after \( N \) steps = \( \langle x^2 \rangle = \langle m^2 \rangle h^2 \).

The quantity \( \sqrt{\langle x^2 \rangle} = \sqrt{\langle m^2 \rangle} h \) is essentially the average distance from the origin after \( N \) steps.

First observe that, from (2.69), we have

\[
\langle m \rangle = 2 \langle k \rangle - N
\]

and

\[
\langle m^2 \rangle = 4 \langle k^2 \rangle - 4 \langle k \rangle N + N^2.
\]

\(^{24}\)The set of walks with \( k \) steps to the right and \( N - k \) to the left is in one to one correspondence with the set of sequences of \( N \) binary digits, containing \( k \) “1” and \( N - k \) “0”, where 1 means *right* and 0 means *left*. There are exactly \( C_{N,k} \) of these sequences.

\(^{25}\)If a random variable \( x \) takes \( N \) possible outcomes \( x_1, \ldots, x_N \) with probability \( p_1, \ldots, p_N \), its **moments of (integer) order** \( q \geq 1 \) are given by

\[
E(x^q) = \langle x^q \rangle = \sum_{j=1}^{N} x_j^q p_j.
\]

The first moment \( (q = 1) \) is the **mean or expected value of** \( x \), while

\[
\text{var}(x) = \langle x^2 \rangle - \langle x \rangle^2
\]

is the **variance of** \( x \). The square root of the variance is called **standard deviation**.
Thus, to compute $\langle m \rangle$ and $\langle m^2 \rangle$ it is enough to compute $\langle k \rangle$ and $\langle k^2 \rangle$. We have, by definition and from (2.71),

$$
\langle k \rangle = \sum_{k=1}^{N} k p_k = \frac{1}{2N} \sum_{k=1}^{N} k C_{N,k}, \quad \langle k^2 \rangle = \sum_{k=1}^{N} k^2 p_k = \frac{1}{2N} \sum_{k=1}^{N} k^2 C_{N,k}. \quad (2.74)
$$

Although it is possible to make the calculations directly from (2.74), it is easier to use the probability generating function, defined by

$$
G(s) = \sum_{k=0}^{N} p_k s^k = \frac{1}{2N} \sum_{k=0}^{N} C_{N,k} s^k.
$$

The function $G$ contains in compact form all the information on the moments of $k$ and works for all the discrete random variables taking integer values. In particular, we have

$$
G'(s) = \frac{1}{2N} \sum_{k=1}^{N} k C_{N,k} s^{k-1}, \quad G''(s) = \frac{1}{2N} \sum_{k=2}^{N} k (k-1) C_{N,k} s^{k-2}. \quad (2.75)
$$

Letting $s = 1$ and using (2.74), we get

$$
G'(1) = \frac{1}{2N} \sum_{k=1}^{N} k C_{N,k} = \langle k \rangle \quad (2.76)
$$

and

$$
G''(1) = \frac{1}{2N} \sum_{k=2}^{N} k (k-1) C_{N,k} = \langle k (k-1) \rangle = \langle k^2 \rangle - \langle k \rangle. \quad (2.77)
$$

On the other hand, letting $a = 1$ and $b = s$ in the elementary formula

$$
(a + b)^N = \sum_{k=0}^{N} C_{N,k} a^{N-k} b^k,
$$

we deduce

$$
G(s) = \frac{1}{2N} (1+s)^N
$$

and therefore

$$
G'(1) = \frac{N}{2} \quad \text{and} \quad G''(1) = \frac{N(N-1)}{4}. \quad (2.78)
$$

From (2.78), (2.76) and (2.77) we easily find

$$
\langle k^2 \rangle = \frac{N}{2} \quad \text{and} \quad \langle k^2 \rangle = \frac{N(N+1)}{4}.
$$

Finally, since $m = 2k - N$, we have

$$
\langle m \rangle = 2 \langle k \rangle - N = 2 \frac{N}{2} - N = 0
$$
and also \( \langle x \rangle = \langle m \rangle h = 0 \), which is not surprising, given the symmetry of the walk. Furthermore

\[
\langle m^2 \rangle = 4 \langle k^2 \rangle - 4N \langle k \rangle + N^2 = N^2 + N - 2N^2 + N^2 = N
\]

from which

\[
\sqrt{\langle x^2 \rangle} = \sqrt{Nh}
\]  

(2.79)

which is the standard deviation of \( x \), since \( \langle x \rangle = 0 \). Formula (2.79) contains a key information: at time \( N\tau \), the distance from the origin is of order \( \sqrt{Nh} \), that is the order of the time scale is the square of the space scale. In other words, if we want to leave the standard deviation unchanged in the limit process, we must rescale the time as the square of the space, that is we must use a space-time parabolic dilation!

But let us proceed step by step. The next one is to deduce a difference equation for the transition probability \( p = p(x, t) \). It is on this equation that we will carry out the limit procedure.

### 2.4.2 The limit transition probability

The particle motion has no memory since each move is independent from the previous one. If the particle location at time \( t + \tau \) is \( x \), this means that at time \( t \) its location was at \( x - h \) or at \( x + h \), with equal probability. The total probability formula then gives

\[
p(x, t + \tau) = \frac{1}{2}p(x - h, t) + \frac{1}{2}p(x + h, t)
\]

(2.80)

with the initial conditions

\[
p(0, 0) = 1 \quad \text{and} \quad p(x, 0) = 0 \quad \text{if} \quad x \neq 0.
\]

Keeping fixed \( x \) and \( t \), let us examine what happens when \( h \to 0, \tau \to 0 \). It is convenient to think of \( p \) as a smooth function, defined in the whole half plane \( \mathbb{R} \times (0, +\infty) \) and not only at the discrete set of points \( (mh, N\tau) \). In addition, by passing to the limit, we will find a continuous probability distribution so that \( p(x, t) \), being the probability to find the particle at \( (x, t) \), should be zero. If we interpret \( p \) as a probability density, this inconvenience disappears. Using Taylor’s formula we can write\(^{26}\)

\[
p(x, t + \tau) = p(x, t) + p_t (x, t) \tau + o(\tau),
\]

\[
p(x \pm h, t) = p(x, t) \pm p_x (x, t) h + \frac{1}{2}p_{xx} (x, t) h^2 + o(h^2).
\]

\(^{26}\) The symbol \( o(z) \), (“little o of \( z \)”) denotes a quantity of lower order with respect to \( z \); precisely

\[
\frac{o(z)}{z} \to 0 \quad \text{when} \quad z \to 0.
\]
Substituting into (2.80), after some simplifications, we find
\[ p_t \tau + o(\tau) = \frac{1}{2} p_{xx} h^2 + o(h^2). \]
Dividing by \( \tau \),
\[ p_t + o(1) = \frac{1}{2} \frac{h^2}{\tau} p_{xx} + o \left( \frac{h^2}{\tau} \right). \quad (2.81) \]
This is the crucial point; in the last equation we meet again the combination \( h^2/\tau \)!!
If we want to obtain something non trivial when \( h, \tau \to 0 \), we must require that \( h^2/\tau \) has a finite and positive limit; the simplest choice is to keep
\[ \frac{h^2}{\tau} = 2D \quad (2.82) \]
for some number \( D > 0 \) (the number 2 is there for aesthetic reasons only).
Passing to the limit in (2.81), we get for \( p \) the equation
\[ p_t = D p_{xx} \quad (2.83) \]
while the initial condition becomes
\[ \lim_{t \to 0^+} p(x, t) = \delta. \quad (2.84) \]
We have already seen that the unique solution of (2.83), (2.84) is
\[ p(x, t) = \Gamma_D(x, t) \]
since
\[ \int_{\mathbb{R}} p(x, t) \, dx = 1. \]
Thus, the constant \( D \) in (2.82) is precisely the diffusion coefficient. Recalling that
\[ h^2 = \frac{\langle x^2 \rangle}{N}, \quad \tau = \frac{t}{N} \]
we have
\[ \frac{h^2}{\tau} = \frac{\langle x^2 \rangle}{t} = 2D \]
that means: in unit time, the particle diffuses an average distance of \( \sqrt{2D} \). It is worthwhile to recall that the dimensions of \( D \) are
\[ [D] = [\text{length}]^2 \times [\text{time}]^{-1} \]
and that the combination \( x^2/Dt \) is dimensionless, not only invariant by parabolic dilations. Also, from (2.82) we deduce
\[ \frac{h}{\tau} = \frac{2D}{h} \to +\infty. \quad (2.85) \]
This shows that the average speed \( h/\tau \) of the particle at each step becomes unbounded. Therefore, the fact that the particle diffuses in unit time to a finite average distance is purely due to the rapid fluctuations of its motion.
2.4.3 From random walk to Brownian motion

What happened in the limit to the random walk? What kind of motion did it become? We can answer using some more tools from probability theory. Let \( x_j = x(j\tau) \) the position of our particle after \( j \) steps and let, for \( j \geq 1 \),

\[
h\xi_j = x_j - x_{j-1}.
\]

The \( \xi_j \) are independent, identically distributed random variables: each one takes on value 1 or \(-1\) with probability \( \frac{1}{2} \). They have expectation \( \langle \xi_j \rangle = 0 \) and variance \( \langle \xi_j^2 \rangle = 1 \). The displacement of the particle after \( N \) steps is

\[
x_N = h \sum_{j=1}^{N} \xi_j.
\]

If we choose

\[
h = \sqrt{\frac{2Dt}{N}},
\]

that is \( \frac{h^2}{\tau} = 2D \), and let \( N \to \infty \), the Central Limit Theorem assures that \( x_N \) converges in law\(^{27}\) to a random variable \( X = X(t) \), normally distributed with mean 0 and variance \( 2Dt \), whose density is \( \Gamma_D(x,t) \).

The random walk has become a continuous walk; if \( D = 1/2 \), it is called (1-dimensional) Brownian motion or Wiener process, that we will characterize later through its essential features.

Usually the symbol \( B = B(t) \) is used to indicate the random position of a Brownian particle. The family of random variables \( B(t) \) (where \( t \) plays the role of a parameter) is defined on a common probability space \( (\Omega, \mathcal{F}, P) \), where \( \Omega \) is the set of elementary events, \( \mathcal{F} \) a \( \sigma \)-algebra in \( \Omega \) of measurable events, and \( P \) a suitable probability measure\(^{28}\) in \( \mathcal{F} \); therefore the right notation should be \( B(t,\omega) \), with \( \omega \in \Omega \), but the dependence on \( \omega \) is usually omitted and understood (for simplicity or laziness).

The family of random variables \( B(t,\omega) \), with time \( t \) as a real parameter, is a continuous stochastic process. Keeping \( \omega \in \Omega \) fixed, we get the real function

\[
t \mapsto B(t,\omega)
\]

whose graph describes a Brownian path (see Fig. 2.8).

\(^{27}\) That is, if \( N \to +\infty \),

\[
\text{Prob}\{a < x_N < b\} \to \int_{a}^{b} \Gamma_D(x,t) \, dx.
\]

\(^{28}\) See Appendix B.
Keeping \( t \) fixed, we get the random variable

\[
\omega \mapsto B(t, \omega).
\]

Without caring too much of what really is \( \Omega \), it is important to be able to compute the probability

\[
P\{B(t) \in I\}
\]

where \( I \subseteq \mathbb{R} \) is a reasonable subset of \( \mathbb{R} \), (a so called Borel set\(^{29}\)). Figure 2.8 shows the meaning of this computation: fixing \( t \) amounts to fixing a vertical straight line, say \( t = \bar{t} \). Let \( I \) be a subset of this line; in the picture \( I \) is an interval. \( P\{B(t) \in I\} \) is the probability that the particle hits \( I \) at time \( t \).

The main properties of Brownian motion are listed below. To be minimalistic we could synthesize everything in the formula\(^{30}\)

\[
dB \sim \sqrt{dt}N(0,1) = N(0,dt)
\]

(2.86)

where \( N(0,1) \) is a normal random variable, with zero mean and variance equal to one.

- **Path continuity.** With probability 1, the possible paths of a Brownian particle are continuous functions

\[
t \mapsto B(t), \quad t \geq 0.
\]

Since from (2.85) the instantaneous speed of the particle is infinite, their graphs are nowhere differentiable!

\(^{29}\) An interval or a set obtained by countable unions and intersections of intervals, for instance. See Appendix B.

\(^{30}\) If \( X \) is a random variable, we write \( X \sim N(\mu, \sigma^2) \) if \( X \) has normal distribution with mean \( \mu \) and variance \( \sigma^2 \).
Gaussian law for increments. We can allow the particle to start from a point \( x \neq 0 \), by considering the process

\[
B^x(t) = x + B(t).
\]

With every point \( x \) is associated a probability \( P^x \), with the following properties (if \( x = 0, P^0 = P \)).

a) \( P^x \{ B^x(0) = x \} = P \{ B(0) = 0 \} = 1 \).

b) For every \( s \geq 0, t \geq 0 \), the increment

\[
B^x(t + s) - B^x(s) = B(t + s) - B(s)
\]

has normal law with zero mean and variance \( t \), whose density is

\[
\Gamma(x,t) \equiv \Gamma_x(x,t) = \frac{1}{\sqrt{2\pi t}} e^{-\frac{x^2}{2t}}.
\]

Moreover it is independent of any event occurred at a time \( \leq s \). For instance, the two events

\[
\{ B^x(t_2) - B^x(t_1) \in I_2 \} \quad \{ B^x(t_1) - B^x(t_0) \in I_1 \}
\]

t_0 < t_1 < t_2, are independent.

- Transition probability. For each Borel set \( I \subseteq \mathbb{R} \), a transition function

\[
P(x,t,I) = P^x \{ B^x(t) \in I \}
\]

is defined, assigning the probability that the particle, initially at \( x \), belongs to \( I \) at time \( t \). We can write:

\[
P(x,t,I) = P \{ B(t) \in I - x \} = \int_{I-x} \Gamma(y,t) \, dy = \int_I \Gamma(y-x,t) \, dy.
\]

- Invariance. The motion is invariant with respect to translations.

- Markov and strong Markov properties. Let \( \mu \) be a probability measure\(^{31} \) on \( \mathbb{R} \). If the initial position of the particle is random with a probability distribution \( \mu \), we can consider a Brownian motion with initial distribution \( \mu \), and for it we use the symbol \( B^\mu \). With this motion is associated a probability distribution \( P^\mu \) such that, for every Borel set \( F \subseteq \mathbb{R} \),

\[
P^\mu \{ B^\mu(0) \in F \} = \mu(F).
\]

The probability that the particle belongs to \( I \) at time \( t \) can be computed through the formula

\[
P^\mu \{ B^\mu(t) \in I \} = \int_{\mathbb{R}} P^x \{ B^x(t) \in I \} \, d\mu(x)
\]

\[
= \int_{\mathbb{R}} P(x,t,I) \, d\mu(x).
\]

\(^{31}\) See Appendix B for the definition of a probability measure \( \mu \) and of the integral with respect to the measure \( \mu \).
The *Markov property* can be stated as follows: given any condition $H$, related to the behavior of the particle before time $s \geq 0$, the process $Y(t) = B^x(t + s)$ is a Brownian motion with initial distribution $\mu(I) = P^x\{B^x(s) \in I \mid H\}$.

This property establishes the independence of the *future* process $B^x(t + s)$ from the *past* (absence of memory) when the *present* $B^x(s)$ is known and reflects the *absence of memory* of the random walk.

In the strong *Markov property*, $s$ is substituted by a random time $\tau$, depending only on the behavior of the particle in the interval $[0, \tau]$. In other words, to decide whether or not the event $\{\tau \leq t\}$ is true, it is enough to know the behavior of the particle up to time $t$. These kinds of random times are called *stopping times*. An important example is the *first exit time* from a domain, that we will consider in the next chapter. Instead, the random time $\tau$ defined by

$$\tau = \inf \{t : B(t) > 10 \text{ and } B(t + 1) < 10\}$$

is not a stopping time. Indeed (measuring time in *seconds*), $\tau$ is “the smallest” among the times $t$ such that the Brownian path is above level 10 at time $t$, and after one second is below 10. Clearly, to decide whether $\tau \leq 3$, say, it is not enough to know the path up to time $t = 3$, since $\tau$ involves the behavior of the path up to the *future* time $t = 4$.

• *Expectation*. Given a sufficiently smooth function $g = g(y), y \in \mathbb{R}$, we can define the random variable

$$Z(t) = (g \circ B^x)(t) = g(B^x(t)).$$

Its expected value is given by the formula

$$E^x[Z(t)] = \int_{\mathbb{R}} g(y) P(x, t, dy) = \int_{\mathbb{R}} g(y) \Gamma(y - x, t) dy.$$ 

We will meet this formula in a completely different situation later on.

## 2.5 Diffusion, Drift and Reaction

### 2.5.1 Random walk with drift

The hypothesis of symmetry of our random walk can be removed. Suppose our unit mass particle moves along the $x$ axis with space step $h > 0$, every time interval of duration $\tau > 0$, according to the following rules (Fig. 2.9).

1. The particle starts from $x = 0$.
2. It moves to the right with probability $p_0 \neq \frac{1}{2}$ and to the left with probability $q_0 = 1 - p_0$, independently of the previous step.
Rule 2 breaks the symmetry of the walk and models a particle tendency to move to the right or to the left, according to the sign of $p_0 - q_0$ being positive or negative, respectively. Again we denote by $p = p(x, t)$ the probability that the particle location is $x = mh$ at time $t = N\tau$. From the total probability formula we have:

$$p(x, t + \tau) = p_0 p(x - h, t) + q_0 p(x + h, t)$$  \hspace{1cm} (2.87)

with the usual initial conditions

$$p(0, 0) = 1 \quad \text{and} \quad p(x, 0) = 0 \quad \text{if} \quad x \neq 0.$$

As in the symmetric case, keeping $x$ and $t$ fixed, we want to examine what happens when we pass to the limit for $h \to 0$, $\tau \to 0$. From Taylor formula, we have

$$p(x, t + \tau) = p(x, t) + p_t(x, t) \tau + o(\tau),$$

$$p(x \pm h, t) = p(x, t) \pm p_x(x, t) h + \frac{1}{2} p_{xx}(x, t) h^2 + o(h^2).$$

Substituting into (2.87), we get

$$p_t \tau + o(\tau) = \frac{1}{2} p_{xx} h^2 + (q_0 - p_0) h p_x + o(h^2).$$ \hspace{1cm} (2.88)

A new term appears: $(q_0 - p_0) h p_x$. Dividing by $\tau$, we obtain

$$p_t + o(1) = \frac{1}{2} \frac{h^2}{\tau} p_{xx} + \left[ \frac{(q_0 - p_0) h}{\tau} p_x \right] + o\left(\frac{h^2}{\tau}\right).$$ \hspace{1cm} (2.89)

Again, here is the crucial point. If we let $h, \tau \to 0$, we realize that the assumption

$$\frac{h^2}{\tau} = 2D$$ \hspace{1cm} (2.90)

alone is not sufficient anymore to get something non trivial from (2.89): indeed, if we keep $p_0$ and $q_0$ constant, we have

$$\frac{(q_0 - p_0) h}{\tau} \to \infty$$

32 $P(A|H)$ denotes the conditional probability of $A$, given $H$. 
and from (2.89) we get a contradiction. What else we have to require? Writing

\[
\frac{(q_0 - p_0) h^2}{\tau} = \frac{(q_0 - p_0) h^2}{h^2} \frac{h}{\tau}
\]

we see we must require, in addition to (2.90), that

\[
\frac{q_0 - p_0}{h} \to \beta \tag{2.91}
\]

with \( \beta \) finite. Notice that, since \( q_0 + p_0 = 1 \), (2.91) is equivalent to

\[
p_0 = \frac{1}{2} - \frac{\beta}{2} h + o(h) \quad \text{and} \quad q_0 = \frac{1}{2} + \frac{\beta}{2} h + o(h),
\]

(2.92)

that could be interpreted as a symmetry of the motion at a microscopic scale.

With (2.91) at hand, we have

\[
\frac{(q_0 - p_0) h^2}{h^2} \frac{h}{\tau} \to 2D\beta \equiv b
\]

and (2.89) becomes in the limit,

\[
p_t = Dp_{xx} + bp_x. \tag{2.93}
\]

We already know that \( Dp_{xx} \) models a diffusion phenomenon. Let us unmask the term \( bp_x \), by first examining the dimensions of \( b \). Since \( q_0 - p_0 \) is dimensionless, being a difference of probabilities, the dimensions of \( b \) are those of \( h/\tau \), namely of a velocity.

Thus the coefficient \( b \) codifies the tendency of the limiting continuous motion, to move towards a privileged direction with speed \( |b| \): to the right if \( b < 0 \), to the left if \( b > 0 \). In other words, there exists a current of intensity \( |b| \) driving the particle. The random walk has become a diffusion process with drift.

The last point of view calls for an analogy with the diffusion of a substance transported along a channel.

### 2.5.2 Pollution in a channel

In this section we examine a simple convection-diffusion model of a pollutant on the surface of a narrow channel. A water stream of constant speed \( v \) transports the pollutant along the positive direction of the \( x \) axis. We can neglect the depth of the water (thinking to a floating pollutant) and the transverse dimension (thinking of a very narrow channel).

Our purpose is to derive a mathematical model capable of describing the evolution of the concentration\(^\text{33}\) \( c = c(x, t) \) of the pollutant. Accordingly, the integral

\[
\int_x^{x+\Delta x} c(y, t) \, dy \tag{2.94}
\]

\(^{33}\) \[c\] = [mass] \times [length]^{-1}.\]
gives the mass inside the interval \([x, x + \Delta x]\) at time \(t\) (Fig. 2.10). In the present case there are neither sources nor sinks of pollutant, therefore to construct a model we use the law of mass conservation: the growth rate of the mass contained in an interval \([x, x + \Delta x]\) equals the net mass flux into \([x, x + \Delta x]\) through the end points.

\[
\frac{d}{dt} \int_{x}^{x+\Delta x} c(y, t) \, dy = \int_{x}^{x+\Delta x} c_t(y, t) \, dy. \tag{2.95}
\]

Denote by \(q = q(x, t)\) the mass flux\(^{35}\) entering the interval \([x, x + \Delta x]\), through the point \(x\) at time \(t\). The net mass flux into \([x, x + \Delta x]\) through the end points is

\[
q(x, t) - q(x + \Delta x, t). \tag{2.96}
\]

Equating (2.95) and (2.96), the law of mass conservation reads

\[
\int_{x}^{x+\Delta x} c_t(y, t) \, dy = q(x, t) - q(x + \Delta x, t).
\]

Dividing by \(\Delta x\) and letting \(\Delta x \to 0\), we find the basic law

\[
c_t = -q_x. \tag{2.97}
\]

At this point we have to decide which kind of mass flux we are dealing with. In other words, we need a constitutive relation for \(q\). There are several possibilities, for instance:

\(^{34}\) Assuming we can take the derivative inside the integral.

\(^{35}\) \([q] = [\text{mass}] \times [\text{time}]^{-1}\)
a) Convection. The flux is determined by the water stream only. This case corresponds to a bulk of pollutant that is driven by the stream, without deformation or expansion. Translating into mathematical terms we find

\[ q(x, t) = vc(x, t) \]

where, we recall, \( v \) denotes the stream speed.

b) Diffusion. The pollutant expands from higher concentration regions to lower ones. We have seen something like that in heat conduction, where, according to the Fourier law, the heat flux is proportional and opposite to the temperature gradient. Here we can adopt a similar law, that in this setting is known as the Fick’s law and reads

\[ q(x, t) = -Dc_x(x, t) \]

where the constant \( D \) depends on the polluting and has the usual dimensions \(|D| = [\text{length}]^2 \times [\text{time}]^{-1}\).

In our case, convection and diffusion are both present and therefore we superpose the two effects, by writing

\[ q(x, t) = vc(x, t) - Dc_x(x, t). \]

From (2.97) we deduce

\[ c_t = Dc_{xx} - vc_x \quad (2.98) \]

which constitutes our mathematical model and turns out to be identical to (2.93).

Since \( D \) and \( v \) are constant, it is easy to determine the evolution of a mass \( Q \) of pollutant, initially located at the origin (say). Its concentration is the solution of (2.98) with initial condition

\[ c(x, 0) = Q\delta(x) \]

where \( \delta \) is the Dirac measure at the origin. To find an explicit formula, we can get rid of the drift term \(-vc_x\) by setting

\[ w(x, t) = c(x, t)e^{hx+kt} \]

with \( h, k \) to be chosen suitably. We have:

\[ w_t = [c_t + kc]e^{hx+kt} \]
\[ w_x = [c_x + hc]e^{hx+kt}, \quad w_{xx} = [c_{xx} + 2hc_x + h^2c]e^{hx+kt}. \]

Using the equation \( c_t = Du_{xx} - vc_x \), we can write

\[ w_t - Dw_{xx} = e^{hx+kt}[c_t - Dc_{xx} - 2Dhc_x + (k - Dh^2)c] = e^{hx+kt}[-v - 2Dh)c_x + (k - Dh^2)c]. \]

Thus if we choose

\[ h = -\frac{v}{2D} \quad \text{and} \quad k = \frac{v^2}{4D}, \]

\[ w(x, t) = e^{hx+kt}c(x, t) \]

where

\[ c(x, t) = Q\delta(x) \]

with \( \delta \) the Dirac measure at the origin.
2.5 Diffusion, Drift and Reaction

$w$ is a solution of the diffusion equation $w_t - Dw_{xx} = 0$, with the initial condition

$$w(x,0) = c(x,0)e^{-\frac{v}{2}x} = Q\delta(x)e^{-\frac{v}{2}x}.$$ 

In chapter 7 we show that $\delta(x)e^{-\frac{v}{2}x} = \delta(x)$, so that $w(x,t) = Q\Gamma_D(x,t)$ and finally

$$c(x,t) = Qe^{\frac{v}{2}x}\Gamma_D(x,t).$$

(2.99)

The concentration $c$ is thus given by the fundamental solution $\Gamma_D$, “carried” by the travelling wave $\exp\left\{\frac{v}{2}D(x - \frac{v}{2}t)\right\}$, in motion to the right with speed $v/2$.

In realistic situations, the pollutant undergoes some sort of decay, for instance by biological decomposition. The resulting equation for the concentration becomes

$$c_t = Dc_{xx} - vc_x - \gamma c$$

where $\gamma$ is a rate of decay$^{36}$. We deal with this case in the next section via a suitable variant of our random walk.

2.5.3 Random walk with drift and reaction

We go back to our 1-dimensional random walk, assuming that the particle loses mass at the constant rate $\gamma > 0$. This means that in an interval of time from $t$ to $t + \tau$ a percentage of mass

$$Q(x,t) = \tau\gamma p(x,t)$$

disappears. The difference equation (2.87) for $p$ becomes

$$p(x,t + \tau) = p_0[p(x-h,t) - Q(x-h,t)] + q_0[p(x+h,t) - Q(x+h,t)]$$

Since$^{37}$

$$p_0Q(x-h,t) + q_0Q(x+h,t) = Q(x,t) + (q_0 - p_0)hQ_x(x,t) + \ldots$$

$$= \tau\gamma p(x,t) + O(\tau h),$$

equation (2.88) modifies into

$$p_t\tau + o(\tau) = \frac{1}{2}p_{xx}h^2 + (q_0 - p_0)hp_x - \tau\gamma p + O(\tau h) + o(h^2).$$

Dividing by $\tau$, letting $h, \tau \to 0$ and assuming

$$\frac{h^2}{\tau} = 2D, \quad \frac{q_0 - p_0}{h} \to \beta,$$

we get

$$p_t = Dp_{xx} + bp_x - \gamma p \quad (b = 2D\beta).$$

(2.100)

$^{36} [\gamma] = \text{[time]}^{-1}$.

$^{37}$ The symbol "$O(k)$" ("big O of k") denotes a quantity of order $k$. 

The term $-\gamma p$ appears in (2.100) as a decaying term. On the other hand, in important situations, $\gamma$ could be negative, meaning that this time we have a creation of mass at the rate $|\gamma|$. For this reason the last term is called generically a reaction term and (2.100) is a diffusion equation with drift and reaction.

Going back to equation (2.100), it is useful to look separately at the effect of the three terms in its right hand side.

- $p_t = D_p x x$ models pure diffusion. The typical effects are spreading and smoothing, as shown by the typical behavior of the fundamental solution $\Gamma_D$.
- $p_t = b p_x$ is a pure transport equation, that we will consider in detail in chapter 3. The solutions are travelling waves of the form $g(x + bt)$.
- $p_t = -\gamma p$ models pure reaction. The solutions are multiples of $e^{-\gamma t}$, exponentially decaying (increasing) if $\gamma > 0$ ($\gamma < 0$).

So far we have given a probabilistic interpretation for a motion in all $\mathbb{R}$, where no boundary condition is present. The problems 7 and 8 give a probabilistic interpretation of the Dirichlet and Neumann condition in terms of absorbing and reflecting boundaries, respectively.

## 2.6 Multidimensional Random Walk

### 2.6.1 The symmetric case

What we have done in dimension $n=1$ can be extended without much effort to dimension $n>1$, in particular $n = 2, 3$. To define a symmetric random walk, we introduce the lattice $\mathbb{Z}^n$ given by the set of points $x \in \mathbb{R}^n$, whose coordinates are signed integers. Given the space step $h > 0$, the symbol $h\mathbb{Z}^n$ denotes the lattice of points whose coordinates are signed integers multiplied by $h$.

Every point $x \in h\mathbb{Z}^n$, has a "discrete neighborhood" of $2n$ points at distance $h$, given by

$x + he_j \quad \text{and} \quad x - he_j \quad (j = 1, ..., n)$,

where $e_1, ..., e_n$ is the canonical basis in $\mathbb{R}^n$. Our particle moves in $h\mathbb{Z}^n$ according to the following rules (Fig. 2.11).

1. It starts from $x = 0$.
2. If it is located in $x$ at time $t$, at time $t + \tau$ the particle location is at one of the $2n$ points $x \pm he_j$, with probability $p = \frac{1}{2n}$.
3. Each step is independent of the previous one.

As in the 1-dimensional case, our task is to compute the probability $p(x, t)$ of finding the particle at $x$ at time $t$.

Clearly the initial conditions for $p$ are

$$p(0, 0) = 1 \quad \text{and} \quad p(x, 0) = 0 \quad \text{if} \ x \neq 0.$$
The total probability formula gives

\[ p(x, t + \tau) = \frac{1}{2n} \sum_{j=1}^{n} \{ p(x + he_j, t) + p(x - he_j, t) \}. \]  

(2.101)

Indeed, to reach the point \( x \) at time \( t + \tau \), at time \( t \) the particle must have been located at one of the points in the discrete neighborhood of \( x \) and moved from there towards \( x \) with probability \( 1/2n \). For fixed \( x \) and \( t \), we want to examine what happens when we let \( h \to 0 \), \( \tau \to 0 \). Assuming \( p \) defined and smooth in all of \( \mathbb{R}^n \times (0, +\infty) \), we use Taylor’s formula to write

\[ p(x, t + \tau) = p(x, t) + p_t(x, t) \tau + o(\tau) \]

\[ p(x \pm he_j, t) = p(x, t) \pm p_{x_j}(x, t) h + \frac{1}{2} p_{x_j x_j}(x, t) h^2 + o(h^2). \]

Substituting into (2.101), after some simplifications, we get

\[ p_t \tau + o(\tau) = \frac{h^2}{2n} \Delta p + o(h^2). \]

Dividing by \( \tau \) we obtain the equation

\[ p_t + o(1) = \frac{1}{2n} \frac{h^2}{\tau} \Delta p + o \left( \frac{h^2}{\tau} \right). \]  

(2.102)

The situation is quite similar to the 1-dimensional case: still, to obtain eventually something non trivial, we must require that the ratio \( h^2/\tau \) has a finite and positive limit. The simplest choice is

\[ \frac{h^2}{\tau} = 2nD \]  

(2.103)
with \(D > 0\). From (2.103), we deduce that in unit time, the particle diffuses at an average distance of \(\sqrt{2nD}\). The physical dimensions of \(D\) have not changed. Letting \(h \to 0, \tau \to 0\) in (2.102), we find for \(p\) the diffusion equation

\[
p_t = D \Delta p
\]

with the initial condition

\[
\lim_{t \to 0^+} p(x, t) = \delta.
\]

Since \(\int_{\mathbb{R}^n} p(x,t) \, dx = 1\) for every \(t\), the unique solution is given by

\[
p(x, t) = \Gamma_D(x, t) = \frac{1}{(4\pi Dt)^{n/2}} e^{-\frac{|x|^2}{4Dt}}, \quad t > 0.
\]

The \(n\)-dimensional random walk has become a continuous walk; when \(D = \frac{1}{2}\), it is called \(n\)-dimensional Brownian motion. Denote by \(B(t) = B(t, \omega)\) the random position of a Brownian particle, defined for every \(t > 0\) on a probability space \((\Omega, \mathcal{F}, P)\).

The family of random variables \(B(t, \omega)\), with time \(t\) as a real parameter, is a vector valued continuous stochastic process. For \(\omega \in \Omega\) fixed, the vector function

\[t \mapsto B(t, \omega)\]

describes an \(n\)-dimensional Brownian path, whose main features are listed below.

- **Path continuity.** With probability 1, the Brownian paths are continuous for \(t \geq 0\).

- **Gaussian law for increments.** The process \(B^x(t) = x + B(t)\) defines a Brownian motion with start at \(x\). With every point \(x\) is associated a probability \(P^x\), with the following properties (if \(x = 0\), \(P^0 = P\)).
  
    a) \(P^x\{B^x(0) = x\} = P\{B(0) = 0\} = 1\).
    
    b) For every \(s \geq 0, t \geq 0\), the increment

    \[
    B^x(t + s) - B^x(s) = B(t + s) - B(s)
    \]

    follows a normal law with zero mean value and covariance matrix equal to \(tI_n\), whose density is

    \[
    \Gamma(x,t) = \Gamma^x_{\frac{n}{2}}(x, t) = \frac{1}{(2\pi t)^{n/2}} e^{-\frac{|x|^2}{2t}}.
    \]

Moreover, (2.106) is independent of any event occurred at any time less than \(s\). For instance, the two events

\[
\{B(t_2) - B(t_1) \in A_1\} \quad \{B(t_1) - B(t_0) \in A_2\}
\]

are independent if \(t_0 < t_1 < t_2\).

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2.6 Multidimensional Random Walk

• **Transition function.** For each Borel set $A \subseteq \mathbb{R}^n$ a transition function

$$P (x, t, A) = P^x \{ B^x (t) \in A \}$$

is defined, representing the probability that the particle, initially located at $x$, belongs to $A$ at time $t$. We have:

$$P (x, t, A) = P \{ B (t) \in A - x \} = \int_{A - x} \Gamma (y, t) \, dy = \int_A \Gamma (y - x, t) \, dy.$$  

• **Invariance.** The motion is invariant with respect to rotations and translations.

• **Markov and strong Markov properties.** Let $\mu$ be a probability measure on $\mathbb{R}^n$. If the particle has a random initial position with probability distribution $\mu$, we can consider a Brownian motion with initial distribution $\mu$, and for it we use the symbol $B^\mu$. To $B^\mu$ is associated a probability distribution $P^\mu$ such that

$$P^\mu \{ B^\mu (0) \in A \} = \mu (A).$$

The probability that the particle belongs to $A$ at time $t$ can be computed through the formula

$$P^\mu \{ B^\mu (t) \in A \} = \int_{\mathbb{R}^n} P (x, t, A) \, d\mu (dx). \quad (2.107)$$

The **Markov property** can be stated as follows: given any condition $H$, related to the behavior of the particle before time $s \geq 0$, the process $Y (t) = B^x (t + s)$, is a Brownian motion with initial distribution

$$\mu (A) = P^x \{ B^x (s) \in A | H \}.$$  

Again, this property establishes the independence of the future process $B^x (t + s)$ from the past when the present $B^x (s)$ is known and encodes the absence of memory of the process. In the strong Markov property, a stopping time $\tau$ takes the place of $s$.

• **Expectation.** Given any sufficiently smooth real function $g = g (y), y \in \mathbb{R}^n$, we can define the real random variable

$$Z (t) = (g \circ B^x) (t) = g (B^x (t)).$$

Its expectation is given by the formula

$$E[Z (t)] = \int_{\mathbb{R}^n} g (y) \, P (x, t, dy) = \int_{\mathbb{R}^n} g (y) \, \Gamma (y - x, t) \, dy.$$  

\(^{39}\) See Appendix B for the definition of a probability measure $\mu$ and of the integral with respect to the measure $\mu$.  

2.6.2 Walks with drift and reaction

As in the 1—dimensional case, we can construct several variants of the symmetric random walk. For instance, we can allow a different behavior along each direction, by choosing the space step $h_j$ depending on $e_j$. As a consequence the limit process models an anisotropic motion, codified in the matrix

$$D = \begin{pmatrix} D_1 & 0 & \cdots & 0 \\ 0 & D_2 & 0 \\ \vdots & \vdots & \ddots \\ 0 & 0 & \cdots & D_n \end{pmatrix}$$

where $D_j = h_j^2 / 2n\tau$ is the diffusion coefficient in the direction $e_j$. The resulting equation for the transition probability $p(x,t)$ is

$$p_t = \sum_{j=1}^{n} D_j p_{x_j x_j}.$$  \hfill (2.108)

We may also break the symmetry by asking that along the direction $e_j$ the probability to go to the left (right) is $q_j$ (resp. $p_j$). If

$$\frac{q_j - p_j}{h_j} \rightarrow \beta_j \quad \text{and} \quad b_j = 2D_j \beta_j,$$

the vector $b = (b_1, ..., b_n)$ plays a role of a drift vector, reflecting the tendency of motion to move asymmetrically along each coordinate axis. Adding a reaction term of the form $cp$, the resulting drift-diffusion-reaction equation is

$$p_t = \sum_{j=1}^{n} D_j p_{x_j x_j} + \sum_{j=1}^{n} b_j u_{x_j} + cp.$$  \hfill (2.109)

In problem 2.17 we ask the reader to fill in all the details in the argument leading to equations (2.108) and (2.109). We will deal with general equations of these type in Chapter 9.

2.7 An Example of Reaction—Diffusion ($n = 3$)

In this section we examine a model of reaction-diffusion in a fissionable material. Although we deal with a greatly simplified model, some interesting implications can be drawn.

By shooting neutrons into an uranium nucleus it may happen that the nucleus breaks into two parts, releasing other neutrons already present in the nucleus and causing a chain reaction. Some macroscopic aspects of this phenomenon can be described by means of an elementary model.
Suppose a cylinder with height $h$ and radius $R$ is made of a fissionable material of constant density $\rho$, with total mass

$$M = \pi \rho R^2 h.$$ 

At a macroscopic level, the free neutrons diffuse like a chemical in a porous medium, with a flux proportional and opposite to the density gradient. In other terms, if $N = N (x, y, z, t)$ is the neutron density and no fission occurs, the flux of neutrons is equal to $-k \nabla N$, where $k$ is a positive constant depending on the material. The mass conservation then gives

$$N_t = k \Delta N.$$ 

When fission occurs at a constant rate $\gamma > 0$, we get the equation

$$N_t = D \Delta N + \gamma N, \quad (2.110)$$

where reaction and diffusion are competing: diffusion tends to slow down $N$, while, clearly, the reaction term tends to exponentially increase $N$. A crucial question is to examine the behavior of $N$ in the long run (i.e. as $t \to +\infty$).

We look for bounded solutions satisfying a homogeneous Dirichlet condition on the boundary of the cylinder, with the idea that the density is higher at the center of the cylinder and very low near the boundary. Then it is reasonable to assume that $N$ has a radial distribution with respect to the axis of the cylinder. More precisely, using the cylindrical coordinates $(r, \theta, z)$ with

$$x = r \cos \theta, \quad y = r \sin \theta,$$

we can write $N = N (r, z, t)$ and the homogeneous Dirichlet condition on the boundary of the cylinder translates into

$$N (R, z, t) = 0 \quad 0 < z < h \quad (2.111)$$

$$N (r, 0, t) = N (r, h, t) = 0 \quad 0 < r < R$$

for every $t > 0$. Accordingly we prescribe an initial condition

$$N (r, z, 0) = N_0 (r, z) \quad (2.112)$$

such that

$$N_0 (R, z) = 0 \text{ for } 0 < z < h, \quad \text{and } N_0 (r, 0) = N_0 (r, h) = 0. \quad (2.113)$$

To solve problem (2.110), (2.111), (2.112), let us first get rid of the reaction term by setting

$$N (r, z, t) = N (r, z, t) e^{\gamma t}. \quad (2.114)$$

Then, writing the Laplace operator in cylindrical coordinates$^{40}$, $\mathcal{N}$ solves

$$\mathcal{N}_t = k \left[ \mathcal{N}_{rr} + \frac{1}{r} \mathcal{N}_r + \mathcal{N}_{zz} \right]$$

$^{40}$ Appendix C.
with the same initial and boundary conditions of $N$. By maximum principle, we know that there exists only one solution, continuous up to the boundary of the cylinder. To find an explicit formula for the solution, we use the method of separation of variables, first searching for bounded solutions of the form

$$ N(r, z, t) = u(r) v(z) w(t), \quad (2.116) $$

satisfying the homogeneous Dirichlet conditions $u(R) = 0$ and $v(0) = v(h) = 0$. Substituting (2.116) into (2.115), we find

$$ u(r) v(z) w'(t) = k[u''(r) v(z) w(t) + \frac{1}{r} u'(r) v(z) w(t) + u(r) v''(z) w(t)]. $$

Dividing by $N$ and rearranging the terms, we get,

$$ \frac{w'(t)}{k w(t)} - \left[ \frac{u''(r)}{u(r)} + \frac{1}{r} \frac{u'(r)}{u(r)} \right] = \frac{v''(z)}{v(z)}. \quad (2.117) $$

The two sides of (2.117) depend on different variables so that they must be equal to a common constant $b$. Then for $v$ we have the eigenvalue problem

$$ v''(z) - bv(z) = 0 $$

$$ v(0) = v(h) = 0. $$

The eigenvalues are $b_m \equiv -\nu_m^2 = -\frac{m^2 \pi^2}{h^2}$, $m \geq 1$ integer, with corresponding eigenfunctions

$$ \nu_m(z) = \sin \nu_m z. $$

The equation for $w$ and $u$ can be written in the form:

$$ \frac{w'(t)}{k w(t)} + \nu_m^2 = \frac{u''(r)}{u(r)} + \frac{1}{r} \frac{u'(r)}{u(r)} \quad (2.118) $$

where the variables $r$ and $t$ are again separated. This forces the two sides of (2.118) to be equal to a common constant $\mu$. Therefore, for $w$ we have the equation

$$ w'(t) = k(\mu - \nu_m^2) w(t) $$

that gives

$$ w(t) = c \exp \left[ k(\mu - \nu_m^2) t \right] \quad c \in \mathbb{R}. \quad (2.119) $$

Then the equation for $u$ is

$$ u''(r) + \frac{1}{r} u'(r) - \mu u(r) = 0 \quad (2.120) $$

with

$$ u(R) = 0 \quad \text{and} \quad u \text{ bounded in } [0, R]. \quad (2.121) $$
The (2.120) is a *Bessel equation of order zero with parameter* $-\mu$; conditions (2.121) force $\mu = -\lambda^2 < 0$. Then the only bounded solution of (2.120), (2.121) is $J_0(\lambda r)$, where

$$J_0(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(k!)^2} \left( \frac{x}{2} \right)^{2k}$$

is the *Bessel function of first kind and order zero*. To match the boundary condition $u(R) = 0$ we require $J_0(\lambda R) = 0$. Now, $J_0$ has an infinite number of positive simple zeros $\lambda_n$, $n \geq 1$:

$$0 < \lambda_1 < \lambda_2 < \ldots < \lambda_n < \ldots$$

Thus, if $\lambda R = \lambda_n$, we find infinitely many solutions of (2.120), given by

$$u_n(r) = J_0 \left( \frac{\lambda_n r}{R} \right).$$

Thus

$$\mu = \mu_n = -\frac{\lambda_n^2}{R^2}.$$  

To summarize, we have determined so far a countable number of solutions

$$\mathcal{N}_{mn}(r, z, t) = u_n(r) v_m(z) w_{m,n}(t) =$$

$$= J_0 \left( \frac{\lambda_n r}{R} \right) \sin v_m z \exp \left[ -k \left( v_m^2 + \frac{\lambda_n^2}{R^2} \right) t \right]$$

satisfying the homogeneous Dirichlet conditions. It remains to satisfy the initial condition. Due to the linearity of the problem, we look for a solution obtained by superposition of the $\mathcal{N}_{m,n}$, that is

$$\mathcal{N}(r, z, t) = \sum_{n,m=1}^{\infty} c_{mn} \mathcal{N}_{mn}(r, z, t).$$

\[41\] In fact, write Bessel’s equation (2.120) in the form

$$(ru')' - \mu ru = 0.$$  

Multiplying by $u$ and integrating over $(0, R)$, we have

$$\int_0^R (ru')' u dr = \mu \int_0^R u^2 dr.$$  \hspace{1cm} (2.122)

Integrating by parts and using (2.121), we get

$$\int_0^R (ru')' u dr = \left[ (ru') u \right]_0^R - \int_0^R (u')^2 dr = - \int_0^R (u')^2 dr < 0$$

and from (2.122) we get $\mu < 0$.

\[42\] The zeros of the Bessel functions are known with a considerable degree of accuracy. The first five zeros of $J_0$ are: 2.4048..., 5.5201..., 8.6537..., 11.7915..., 14.9309....
Then, we choose the coefficients $c_{mn}$ in order to have

$$\sum_{n,m=1}^{\infty} c_{mn} N_{mn}(r, z, 0) = \sum_{n,m=1}^{\infty} c_{mn} J_0 \left( \frac{\lambda_n r}{R} \right) \sin \frac{m\pi}{h} z = N_0(r, z). \quad (2.123)$$

The second of (2.113) and (2.123) suggest an expansion of $N_0$ in sine Fourier series with respect to $z$. Let

$$c_m(r) = \frac{2}{h} \int_0^h N(r, z) \sin \frac{m\pi}{h} z, \quad m \geq 1,$$

and

$$N_0(r, z) = \sum_{m=1}^{\infty} c_m(r) \sin \frac{m\pi}{h} z.$$

Then (2.123) shows that, for fixed $m \geq 1$, the $c_{mn}$ are the coefficients of the expansion of $c_m(r)$ in the Fourier-Bessel series

$$\sum_{n=1}^{\infty} c_{mn} J_0 \left( \frac{\lambda_n r}{R} \right) = c_m(r).$$

We are not really interested in the exact formula for the $c_{mn}$, however we will come back to this point in Remark 2.5 below.

In conclusion, recalling (2.114), the analytic expression of the solution of our original problem is the following:

$$N(r, z, t) = \sum_{n,m=1}^{\infty} c_{mn} J_0 \left( \frac{\lambda_n r}{R} \right) \exp \left\{ \left( \gamma - k\nu_m^2 - k\frac{\lambda_n^2}{R^2} \right) t \right\} \sin m\pi \frac{z}{2}. \quad (2.124)$$

Of course, (2.124) is only a formal solution, since we should check in which sense the boundary and initial condition are attained and that term by term differentiation can be performed. This can be done under reasonable smoothness properties of $N_0$ and we do not pursue the calculations here.

Rather, we notice that from (2.124) we can draw an interesting conclusion on the long range behavior of $N$. Consider for instance the value of $N$ at the center of the cylinder, that is at the point $r = 0$ and $z = h/2$; we have, since $J_0(0) = 1$ and $\nu_m^2 = \frac{m^2\pi^2}{h^2}$,

$$N \left( 0, \frac{h}{2}, t \right) = \sum_{n,m=1}^{\infty} c_{mn} \exp \left\{ \left( \gamma - k\frac{m^2\pi^2}{h^2} - k\frac{\lambda_n^2}{R^2} \right) t \right\} \sin \frac{m\pi}{2}.$$

The exponential factor is maximized for $m = n = 1$, so the leading term in the sum is

$$c_{11} \exp \left\{ \left( \gamma - k\frac{\pi^2}{h^2} - k\frac{\lambda_1^2}{R^2} \right) t \right\}.$$
If now
\[ \gamma - k \left( \frac{\pi^2}{h^2} + \frac{\lambda_1^2}{R^2} \right) < 0, \]
each term in the series goes to zero as \( t \to +\infty \) and the reaction dies out. On the opposite, if
\[ \gamma - k \left( \frac{\pi^2}{h^2} + \frac{\lambda_1^2}{R^2} \right) > 0, \]
that is
\[ \frac{\gamma}{k} > \frac{\pi^2}{h^2} + \frac{\lambda_1^2}{R^2}, \] (2.125)
the leading term increases exponentially with time. To be true, (2.125) requires that the following relations be both satisfied:
\[ h^2 > \frac{k\pi^2}{\gamma} \quad \text{and} \quad R^2 > \frac{k\lambda_1^2}{\gamma}. \] (2.126)

The (2.126) gives a lower bound for the height and the radius of the cylinder. Thus, we deduce that there exists a critical mass of material, below which the reaction cannot be sustained.

**Fig. 2.12.** The Bessel function \( J_0 \)

*Remark 2.5.* A sufficiently smooth function \( f \), for instance of class \( C^1([0, R]) \), can be expanded in a Fourier-Bessel series, where the Bessel functions \( J_0 \left( \frac{\lambda_n r}{R} \right) \), \( n \geq 1 \), play the same role of the trigonometric functions. More precisely, the functions \( J_0(\lambda_n r) \) satisfy the following orthogonality relations:
\[ \int_0^R x J_0(\lambda_m x) J_0(\lambda_n x) dx = \begin{cases} 0 & m \neq n \\ \frac{R^2}{2} c_n^2 & m = n \end{cases} \]
where
\[ c_n = \sum_{k=0}^{\infty} \frac{(-1)^k}{k! (k+1)!} \left( \frac{\lambda_n}{2R} \right)^{2k+1}. \]
Then
\[ f(x) = \sum_{n=0}^{\infty} f_n J_0(\lambda_n x) \] (2.127)

with the coefficients \(f_n\) assigned by the formula
\[ f_n = \frac{2}{R^2 e^2_n} \int_{0}^{R} x f(x) J_0(\lambda_n x) \, dx. \]

The series (2.127) converges in the following least square sense: if
\[ S_N(x) = \sum_{n=0}^{N} f_n J_0(\lambda_n x) \]
then
\[ \lim_{N \to +\infty} \int_{0}^{R} [f(x) - S_N(x)]^2 \, dx = 0. \] (2.128)

In Chapter 6, we will interpret (2.128) from the point of view of Hilbert space theory.

### 2.8 The Global Cauchy Problem \( (n = 1) \)

#### 2.8.1 The homogeneous case

In this section we consider the global Cauchy problem
\[ \begin{align*}
  u_t - Du_{xx} &= 0 \quad \text{in } \mathbb{R} \times (0, \infty) \\
  u(x, 0) &= g(x) \quad \text{in } \mathbb{R}
\end{align*} \] (2.129)

where \(g\), the initial data, is given. We will limit ourselves to the one dimensional case; techniques, ideas and formulas can be extended without too much effort to the \(n\)-dimensional case.

The problem (2.129) models the evolution of the temperature or of the concentration of a substance along a very long (infinite) bar or channel, respectively, given the initial \((t = 0)\) distribution.

By heuristic considerations, we can guess what could be a candidate solution. Consider a unit mass composed of a large number \(M \gg 1\) of particles and interpret the solution \(u\) as their concentration (or percentage). Then, \(u(x,t) \, dx\) gives the mass inside the interval \((x, x + dx)\) at time \(t\).

We want to determine the concentration \(u(x,y)\), due to the diffusion of a mass whose initial concentration is given by \(g\).

Thus, the quantity \(g(y) \, dy\) represents the mass concentrated in the interval \((y, y + dy)\) at time \(t = 0\). As we have seen, \(\Gamma(x - y, t)\) is a unit source solution,
representing the concentration at \( x \) at time \( t \), due to the diffusion of a unit mass, initially concentrated in the same interval. Accordingly,

\[ \Gamma_D (x - y, t) g(y) \, dy \]

gives the concentration at \( x \) at time \( t \), due to the diffusion of the mass \( g(y) \, dy \).

Thanks to the linearity of the diffusion equation, we can use the superposition principle and compute the solution as the sum of all contributions. In this way, we get the formula

\[
  u(x, t) = \int_{\mathbb{R}} g(y) \Gamma_D (x - y, t) \, dy = \frac{1}{\sqrt{4\pi Dt}} \int_{\mathbb{R}} g(y) e^{-\frac{(x-y)^2}{4Dt}} \, dy. \tag{2.130}
\]

Clearly, one has to check rigorously that, under reasonable hypotheses on the initial data \( g \), formula (2.130) really gives the unique solution of the Cauchy problem. This is not a negligible question. First of all, if \( g \) grows too much at infinity, more than an exponential of the type \( e^{ax^2}, a > 0 \), in spite of the rapid convergence to zero of the Gaussian, the integral in (2.130) could be divergent and formula (2.130) loses any meaning. Even more delicate is the question of the uniqueness of the solution, as we will see later.

Remark 2.6. Formula (2.130) has a probabilistic interpretation. Let \( D = \frac{1}{2} \) and let \( B^x (t) \) be the position of a Brownian particle, started at \( x \). Let \( g(y) \) be the gain obtained when the particle crosses \( y \). Then, we can write:

\[ u(x, t) = E^x [g(B^x(t))] \]

where \( E^x \) denotes the expected value with respect to the probability \( P^x \), with density \( \Gamma(x - y, t) \).

In other words: to compute \( u \) at the point \((x, t)\), consider a Brownian particle starting at \( x \), compute its position \( B^x(t) \) at time \( t \), and finally compute the expected value of \( g(B^x(t)) \).

### 2.8.2 Existence of a solution

The following theorem states that (2.130) is indeed a solution of the global Cauchy problem under rather general hypotheses on \( g \), satisfied in most of the interesting applications\(^{44}\).

**Theorem 2.3.** Assume that \( g \) is a function with a finite number of jump discontinuities in \( \mathbb{R} \) and there exist positive numbers \( a \) and \( c \) such that

\[ |g(x)| \leq ce^{ax^2} \quad \forall x \in \mathbb{R}. \tag{2.131} \]

\(^{43}\) Appendix B.

\(^{44}\) We omit the long and technical proof.
Let \( u \) be given by formula (2.130). Then:

i) \( u \in C^\infty (\mathbb{R} \times (0, T)) \) for \( T < \frac{1}{4Da} \), and in the strip \( \mathbb{R} \times (0, T) \)
\[ u_t - Du_{xx} = 0. \]

ii) If \( x_0 \) is a continuity point of \( g \), then
\[ u (y, t) \to g (x_0) \quad \text{if} \quad (y, t) \to (x_0, 0), t > 0. \]

iii) There are positive numbers \( c_1 \) and \( A \) such that
\[ |u (x, t)| \leq Ce^{Ax^2} \quad \forall (x, t) \in \mathbb{R} \times (0, \infty). \]

**Remark 2.7.** The theorem says that, if we allow an initial data with a controlled exponential growth at infinity expressed by (2.131), then (2.130) is a solution in the strip \( \mathbb{R} \times (0, T) \). We will see that, under the stated conditions, (2.130) is actually the unique solution.

In some applications (e.g. to Finance), the initial data grows at infinity no more than \( c_1 e^{a_1 |x|} \). In this case (2.131) is satisfied by choosing any positive number \( a \) and a suitable \( c \). This means that there is really no limitation on \( T \), since
\[ T < \frac{1}{4Da} \]
and \( a \) can be chosen as small as we like.

**Remark 2.8.** The property \( i) \) shows a typical and important phenomenon connected with the diffusion equation: even if the initial data is discontinuous at some point, immediately after the solution is smooth. The diffusion is therefore a smoothing process. In figure 2.13, this phenomenon is shown for the initial data \( g (x) = \chi_{(-2, 0)} (x) + \chi_{(1, 4)} (x) \), where \( \chi_{(a,b)} \) denotes the characteristic function of the interval \( (a,b) \). By \( ii) \), if the initial data \( g \) is continuous in all of \( \mathbb{R} \), then the solution is continuous up to \( t = 0 \), that is in \( \mathbb{R} \times [0, T) \).

![Fig. 2.13. Smoothing effect of the diffusion equation](image-url)
2.8.3 The non homogeneous case. Duhamel's method

The difference equation (or the total probability formula)

\[ p(x, t + \tau) = \frac{1}{2} p(x - h, t) + \frac{1}{2} p(x + h, t) \]

that we found in subsection 2.4.2 during the analysis of the symmetric random walk could be considered a probabilistic version of the mass conservation principle: the density of the mass located at \( x \) at time \( t + \tau \) is the sum of the densities diffused from \( x + h \) and \( x - h \) at time \( t \); no mass has been lost or added over the time interval \([t, t + \tau] \). Accordingly, the expression

\[ p(x, t + \tau) - \left[ \frac{1}{2} p(x - h, t) + \frac{1}{2} p(x + h, t) \right] \] (2.132)

could be considered as a measure of the lost/added mass density over the time interval from \( t \) to \( t + \tau \). Expanding with Taylor’s formula as we did in Section 4.2, keeping \( h^2/\tau = 2D \), dividing by \( \tau \) and letting \( h, \tau \to 0 \) in (2.132), we find

\[ p_t - Dp_{xx}. \]

Thus the differential operator \( \partial_t - D\partial_{xx} \) measures the instantaneous density production rate.

Suppose now that from time \( t = 0 \) until a certain time \( t = s > 0 \) no mass is present and that at time \( s \) a unit mass at the point \( y \) (infinite density) appears. We know we can model this kind of source by means of a Dirac measure at \( y \), that has to be time dependent since the mass appears only at time \( s \). We can write it in the form

\[ \delta(x - y, t - s). \]

Thus, we are lead to the non homogeneous equation

\[ p_t - Dp_{xx} = \delta(x - y, t - s) \]

with \( p(x, 0) = 0 \) as initial condition. What could be the solution? Until \( t = s \) nothing happens and after \( s \) we have \( \delta(x - y, t - s) = 0 \). Therefore it is like starting from time \( t = s \) and solving the problem

\[ p_t - Dp_{xx} = 0, \quad x \in \mathbb{R}, \ t > s \]

with initial condition

\[ p(x, s) = \delta(x - y, t - s). \]

We have solved this problem when \( s = 0 \); the solution is \( \Gamma_D(x - y, t) \). By the time translation invariance of the diffusion equation, we deduce that the solution for any \( s > 0 \) is given by

\[ p(x, t) = \Gamma_D(x - y, t - s). \] (2.133)
Consider now a distributed source on the half-plane \( t > 0 \), capable to produce mass density at the time rate \( f(x, t) \). Precisely, \( f(x, t) \, dx \, dt \) is the mass produced\(^{45}\) between \( x \) and \( x + dx \), over the time interval \( (t, t + dt) \). If initially no mass is present, we are lead to the non homogeneous Cauchy problem

\[
\begin{cases}
  v_t - Dv_{xx} = f(x, t) & \text{in } \mathbb{R} \times (0, T) \\
  v(x, 0) = 0 & \text{in } \mathbb{R}.
\end{cases}
\] (2.134)

As in subsection 2.8.1, we motivate the form of the solution at the point \((x, t)\) using heuristic considerations. Let us compute the contribution \( dv \) to \( v(x, t) \) of a mass \( f(y, s) \, dy \, ds \). It is like having a source term of the form

\[
f^* (x, t) = f(x, t) \delta(x - y, t - s)
\]

and therefore, recalling (2.133), we have

\[
dv(x, t) = \Gamma_D(x - y, t - s) f(y, s) \, dy \, ds.
\] (2.135)

We obtain the solution \( v(x, t) \) by superposition, summing all the contributions (2.135). We split it into the following two steps:

- we sum over \( y \) the contributions for fixed \( s \), to get the total density at \((x, t)\), due to the diffusion of mass produced at time \( s \). The result is \( w(x, t, s) \, ds \), where

\[
w(x, t, s) = \int_{\mathbb{R}} \Gamma_D(x - y, t - s) f(y, s) \, dy.
\] (2.136)

- we sum the above contributions for \( s \) ranging from 0 to \( t \):

\[
v(x, t) = \int_0^t \int_{\mathbb{R}} \Gamma_D(x - y, t - s) f(y, s) \, dy \, ds.
\]

The above construction is an example of application of the Duhamel method, that we state below:

**Duhamel's method.** The procedure to solve problem (2.134) consists in the following two steps:

1. Construct a family of solutions of homogeneous Cauchy problems, with variable initial time \( s > 0 \), and initial data \( f(x, s) \).

2. Integrate the above family with respect to \( s \), over \((0, t)\).

Indeed, let us examine the two steps.

1. Consider the homogeneous Cauchy problems

\[
\begin{cases}
  w_t - Dw_{xx} = 0 & x \in \mathbb{R}, \ t > s \\
  w(x, s, s) = f(x, s) & x \in \mathbb{R}
\end{cases}
\] (2.137)

where the initial time \( s \) plays the role of a parameter.

\(^{45}\) Negative production \((f < 0)\) means removal.
The function $\Gamma_{y,s} (x,t) = \Gamma_D (x-y,t-s)$ is the fundamental solution of the diffusion equation that satisfies for $t = s$, the initial condition

$$\Gamma_{y,s} (x,s) = \delta (x-y).$$

Hence, the solution of (2.137) is given by the function (2.136):

$$w (x,t,s) = \int_{\mathbb{R}} \Gamma_D (x-y,t-s) f (y,s) \, dy.$$

Thus, $w (x,t,s)$ is the required family.

2. Integrating $w$ over $(0,t)$ with respect to $s$, we find

$$v (x,t) = \int_0^t w (x,t,s) \, ds = \int_0^t \int_{\mathbb{R}} \Gamma_D (x-y,t-s) f (y,s) \, dy \, ds. \quad (2.138)$$

Using (2.137) we have

$$v_t - Dv_{xx} = w (x,t,t) + \int_0^t [w_t (x,t,s) - Dw_{xx} (x,t,s)] = f (x,t).$$

Moreover, $v (x,0) = 0$ and therefore $v$ is a solution to (2.134).

Everything works under rather mild hypotheses on $f$. More precisely:

**Theorem 2.4.** If $f$ and its derivatives $f_t, f_x, f_{xx}$ are continuous and bounded in $\mathbb{R} \times [0,T)$, then (2.138) gives a solution $v$ of problem (2.134) in $\mathbb{R} \times (0,T)$, continuous up to $t = 0$, with derivatives $v_t, v_x, v_{xx}$ continuous in $\mathbb{R} \times (0,T)$.

The formula for the general Cauchy problem

$$\begin{cases}
  u_t - Du_{xx} = f (x,t) & \text{in } \mathbb{R} \times (0,T) \\
  u (x,0) = g (x) & \text{in } \mathbb{R}
\end{cases} \quad (2.139)$$

is obtained by superposition of (2.130) and (2.134):

$$u (x,t) = \int_{\mathbb{R}} \Gamma_D (x-y,t) g (y) \, dy + \int_0^t \int_{\mathbb{R}} \Gamma (x-y,t-s) f (y,s) \, dy \, ds \quad (2.140)$$

Under the hypotheses on $f$ and $g$ stated in Theorems 2.3 and 2.4, (2.140) is a solution of (2.139) in $\mathbb{R} \times (0,T)$, continuous with its derivatives $u_t, u_x, u_{xx}$.

The initial condition means that $u (x,t) \to g (x_0)$ as $(x,t) \to (x_0,0)$ at any point $x_0$ of continuity of $g$. In particular, if $g$ is continuous in $\mathbb{R}$ then $u$ is continuous in $\mathbb{R} \times [0,T)$.
2.8.4 Maximum principles and uniqueness

The uniqueness of the solution to the global Cauchy problem is still to be discussed. This is not a trivial question since the following counterexample of Tychonov shows that there could be several solutions of the homogeneous problem. Let

\[
h(t) = \begin{cases} \ e^{-t^2} & \text{for } t > 0 \\ 0 & \text{for } t \leq 0. \end{cases}
\]

It can be checked\(^{46}\) that the function

\[
T(x, t) = \sum_{k=0}^{\infty} \frac{x^{2k}}{(2k)!} \frac{d^k}{dt^k} h(t)
\]

is a solution of

\[
u_t - u_{xx} = 0 \quad \text{in } \mathbb{R} \times (0, +\infty)
\]

with

\[
u(x, 0) = 0 \quad \text{in } \mathbb{R}.
\]

Since also \(u(x, t) \equiv 0\) is a solution of the same problem, we conclude that, in general, the Cauchy problem is not well posed.

What is wrong with \(T\)? It grows too much at infinity for small times. Indeed the best estimate available for \(T\) is the following:

\[
|T(x, t)| \leq C \exp \left\{ \frac{x^2}{\theta t} \right\} \quad (\theta > 0)
\]

that quickly deteriorates when \(t \to 0^+\), due to the factor \(1/\theta t\).

If instead of \(1/\theta t\) we had a constant \(A\), as in condition (iii) of Theorem 2.3, then we can assure uniqueness.

In other words, among the class of functions with growth at infinity controlled by an exponential of the type \(Ce^{Ax^2}\) for any \(t \geq 0\) (the so called Tychonov class), the solution to the homogeneous Cauchy problem is unique.

This is a consequence of the following maximum principle.

**Theorem 2.5 (Global maximum principle).** Let \(z\) be continuous in \(\mathbb{R} \times [0, T]\), with derivatives \(z_x, z_{xx}, z_t\) continuous in \(\mathbb{R} \times (0, T)\), such that, in \(\mathbb{R} \times (0, T)\):

\[
z_t - Dz_{xx} \leq 0 \quad (\text{resp. } \geq 0)
\]

and

\[
z(x, t) \leq Ce^{Ax^2}, \quad (\text{resp. } \geq -Ce^{Ax^2}) \quad (2.141)
\]

where \(C > 0\). Then

\[
\sup_{\mathbb{R} \times [0, T]} z(x, t) \leq \sup_{\mathbb{R}} z(x, 0) \quad (\text{resp. } \inf_{\mathbb{R} \times [0, T]} z(x, t) \geq \inf_{\mathbb{R}} z(x, 0)).
\]

\(^{46}\) Not an easy task! See John’s book in the references.
The proof is rather difficult, but if we assume that \( z \) is bounded from above or below \((A = 0 \text{ in } (2.141))\), then the proof relies on a simple application of the weak maximum principle, Theorem 2.2.

In Problem 2.13 we ask the reader to fill in the details of the proof.

We now are in position to prove the following uniqueness result.

**Corollary 2.2.** Uniqueness I. Suppose \( u \) is a solution of

\[
\begin{align*}
  u_t - Du_{xx} &= 0 \text{ in } \mathbb{R} \times (0, T) \\
  u(x, 0) &= 0 \text{ in } \mathbb{R},
\end{align*}
\]

continuous in \( \mathbb{R} \times [0, T] \), with derivatives \( u_x, u_{xx}, u_t \) continuous in \( \mathbb{R} \times (0, T) \). If \( |u| \) satisfies \((2.141)\) then \( u \equiv 0 \).

**Proof.** From Theorem 2.5 we have

\[
0 = \inf_{\mathbb{R}} u(x, 0) \leq \inf_{\mathbb{R} \times [0, T]} u(x, t) \leq \sup_{\mathbb{R} \times [0, T]} u(x, t) \leq \sup_{\mathbb{R}} u(x, 0) = 0
\]

so that \( u \equiv 0 \). \( \square \)

Notice that if

\[|g(x)| \leq ce^{ax^2} \quad \text{for every } x \in \mathbb{R} \quad (c, a \text{ positive}), \tag{2.142}\]

we know from Theorem 2.3 that

\[u(x, t) = \int_{\mathbb{R}} \Gamma_D(x - y, t) g(y) \, dy\]

satisfies the estimate

\[|u(x, t)| \leq Ce^{Ax^2} \quad \text{in } \mathbb{R} \times (0, T) \tag{2.143}\]

and therefore it belongs to the Tychonov class in \( \mathbb{R} \times (0, T) \), for \( T < 1/4Da \).

Moreover, if \( f \) is as in Theorem 2.4 and

\[v(x, t) = \int_{0}^{t} \int_{\mathbb{R}} \Gamma_D(x - y, t - s) f(y, s) \, dy \, ds,\]

we easily get the estimate

\[t \inf_{\mathbb{R}} f \leq v(x, t) \leq t \sup_{\mathbb{R}} f, \tag{2.144}\]

for every \( x \in \mathbb{R}, 0 \leq t \leq T \). In fact:

\[v(x, t) \leq \sup_{\mathbb{R}} f \int_{0}^{t} \int_{\mathbb{R}} \Gamma_D(x - y, t - s) \, dy \, ds = t \sup_{\mathbb{R}} f\]

since

\[\int_{\mathbb{R}} \Gamma_D(x - y, t - s) \, dy = 1\]

for every \( x, t, s, t > s \). In the same way it can be shown that \( v(x, t) \geq t \inf_{\mathbb{R}} f \).

As a consequence, we have:
Corollary 2.3. Uniqueness II. Let $g$ be continuous in $\mathbb{R}$, satisfying (2.143), and let $f$ be as in Theorem 2.4. Then the Cauchy problem (2.139) has a unique solution $u$ in $\mathbb{R} \times (0, T)$ for $T < 1/4Da$, belonging to the Tychonov class. This solution is given by (2.140) and moreover

$$\inf_{\mathbb{R}} g + t \inf_{\mathbb{R}} f \leq u(x, t) \leq \sup_{\mathbb{R}} g + t \sup_{\mathbb{R}} f. \quad (2.145)$$

Proof. If $u$ and $v$ are solutions of the same Cauchy problem (2.139), then $w = u - v$ is a solution of (2.139) with $f = g = 0$ and satisfies the hypotheses of Corollary 2.2. It follows that $w(x, t) \equiv 0$. □

- Stability and comparison. As in Corollary 2.1, inequality (2.145) is a stability estimate for the correspondence

$$data \mapsto solution.$$ 

Indeed, let $u_1$ and $u_2$ be solutions of (2.139) with data $g_1, f_1$ and $g_2, f_2$, respectively. Under the hypotheses of Corollary 2.2, from (2.145) we can write

$$\sup_{\mathbb{R} \times [0, T]} |u_1 - u_2| \leq \sup_{\mathbb{R}} |g_1 - g_2| + T \sup_{\mathbb{R} \times [0, T]} |f_1 - f_2|.$$ 

Therefore if

$$\sup_{\mathbb{R} \times [0, T]} |f_1 - f_2| \leq \varepsilon, \quad \sup_{\mathbb{R}} |g_1 - g_2| \leq \varepsilon$$

also

$$\sup_{\mathbb{R} \times [0, T]} |u_1 - u_2| \leq \varepsilon (1 + T)$$

that means uniform pointwise stability.

This is not the only consequence of (2.145). We can use it to compare two solutions. For instance, from the left inequality we immediately deduce that if $f \geq 0$ and $g \geq 0$, also $u \geq 0$.

Similarly, if $f_1 \geq f_2$ and $g_1 \geq g_2$, then

$$u_1 \geq u_2.$$ 

- Backward equations arise in several applied contexts, from control theory and dynamic programming to probability and finance. An example is the celebrated Black–Scholes equation we will present in the next section.

Due to the time irreversibility, to have a well posed problem for the backward equation in the time interval $[0, T]$ we must prescribe a final condition, that is for $t = T$, rather than an initial one. On the other hand, the change of variable $t \mapsto T - t$ transforms the backward into the forward equation, so that, from the mathematical point of view, the two equations are equivalent. Except for this remark the theory we have developed so far remains valid.
2.9 An Application to Finance

2.9.1 European options

In this section we apply the above theory to determine the price of some financial products, in particular of some derivative products, called European options.

A financial product is a derivative if its payoff depends on the price behavior of an asset, in jargon the underlying, for instance a stock, a currency or a commodity.

Among the simplest derivatives are the European call and put options, that are contracts on a prescribed asset between a holder and a subscriber, with the following rules.

At the drawing up time of the contract (say at time $t = 0$) an exercise or strike price $E$ is fixed.

At an expiry date $T$, fixed in the future,

- the holder of a call option can (but is not obliged to) exercise the option by purchasing the asset at the price $E$. If the holder decides to buy the asset, the subscriber must sell it;
- the holder of a put option can (but is not obliged to) exercise the option by selling at the price $E$. If the holder decides to sell the asset, the subscriber must buy it.

Since an option gives to the holder a right without any obligation, the option has a price and the basic question is: what is the “right” price that must be paid at $t = 0$?

This price certainly depends on the evolution of the price $S$ of the underlying, on the strike price $E$, on the expiring time $T$ and on the current riskless interest rate $r > 0$.

For instance, for a call, to a lower $E$ corresponds a greater price; the opposite holds for a put. The price fluctuations of the underlying affect in crucial way the value of an option, since they incorporate the amount of risk.

To answer our basic question, we introduce the value function $V = V(S, t)$, giving the proper price of the option if at time $t$ the price of the underlying is $S$. What we need to know is $V(S(0), 0)$. When we like to distinguish between call and put, we use the notations $C(S, t)$ and $P(S, t)$, respectively.

The problem is then to determine $V$ in agreement with the financial market, where both the underlying and the option are exchanged. We shall use the Black-Scholes method, based on the assumption of a reasonable evolution model for $S$ and on the fundamental principle of no arbitrage possibilities.

2.9.2 An evolution model for the price $S$

Since $S$ depends on more or less foreseeable factors, it is clear that we cannot expect a deterministic model for the evolution of $S$. To construct it we assume a market efficiency in the following sense:
a) The market responds instantaneously to new information on the asset.
b) The price has no memory: its past history is fully stored in the present price, without further information.

Condition a) implies the adoption of a continuous model. Condition b) basically requires that a change \( dS \) of the underlying price has the Markov property, like Brownian motion.

Consider now a time interval from \( t \) to \( t + dt \), during which \( S \) undergoes a change from \( S \) to \( S + dS \). One of the most common models assumes that the \textbf{return} \( dS/S \) is given by the sum of two terms.

One is a deterministic term, which gives a contribution \( \mu dt \) due to a constant \textit{drift} \( \mu \), representing the average growth rate of \( S \). With this term alone, we would have

\[
\frac{dS}{S} = \mu dt
\]

and therefore \( d\log S = \mu dt \), that gives the exponential growth \( S(t) = S(0)e^{\mu t} \).

The other term is stochastic and takes into account the random aspects of the evolution. It gives the contribution

\[
\sigma dB
\]

where \( dB \) is an increment of a Brownian motion and has zero mean and variance \( dt \). The coefficient \( \sigma \), that we assume to be constant, is called the \textbf{volatility} and measures the standard deviation of the return.

Summing the contributions we have

\[
\frac{dS}{S} = \mu dt + \sigma dB. \tag{2.146}
\]

Note the physical dimensions of \( \mu \) and \( \sigma \): \( [\mu] = [\text{time}]^{-1}, [\sigma] = [\text{time}]^{-\frac{1}{2}} \).

The (2.146) is a \textbf{stochastic differential equation} (s.d.e.). To solve it one is tempted to write

\[
d\log S = \mu dt + \sigma dB,
\]

to integrate between 0 e \( t \), and to obtain

\[
\log \frac{S(t)}{S(0)} = \mu t + \sigma (B(t) - B(0)) = \mu t + \sigma B(t)
\]

since \( B(0) = 0 \). However, this is not correct. The diffusion term \( \sigma dB \) requires the use of the \textbf{Itô formula}, a stochastic version of the chain rule. Let us make a few intuitive remarks on this important formula.

\textit{Digression on Itô’s formula.} Let \( B = B(t) \) the usual Brownian motion. An Itô process \( X = X(t) \) is a solution of a s.d.e. of the type

\[
dX = a(X, t)dt + \sigma(X, t)dB \tag{2.147}
\]

where \( a \) is the \textit{drift term} and \( \sigma \) is the \textbf{volatility coefficient}.
When \( \sigma = 0 \), the equation is deterministic and the trajectories can be computed with the usual analytic methods. Moreover, given a smooth function \( F = F(x,t) \), we can easily compute the variation of \( F \) along those trajectories. It is enough to compute
\[
dF = F_t dt + F_x dX = \{ F_t + aF_x \} dt.
\]
Let now be \( \sigma \) non zero; the preceding computation would give
\[
dF = F_t dt + F_x dX = \{ F_t + aF_x \} dt + \sigma F_x dB
\]
but this formula does not give the complete differential of \( F \). Indeed, using Taylor’s formula, one has, letting \( X(0) = X_0 \):
\[
F(X,t) = F(X_0,0) + F_t dt + F_x dX + \frac{1}{2} \left\{ F_{xx} (dX)^2 + 2F_{xt} dXdX + F_{tt} (dt)^2 \right\} + \ldots.
\]
The differential of \( F \) along the trajectories of (2.147) is obtained by selecting in the right hand side of the preceding formula the terms which are linear with respect to \( dt \) or \( dX \). We first find the terms
\[
F_t dt + F_x dX = \{ F_t + aF_x \} dt + \sigma F_x dB.
\]
The terms \( 2F_{xt} dX dt \) and \( F_{tt} (dt)^2 \) are non linear with respect to \( dt \) and \( dX \) and therefore they are not in the differential. Let us now check the term \( (dX)^2 \). We have
\[
(dX)^2 = [adt + \sigma dB]^2 = a^2 (dt)^2 + 2a\sigma dB dt + \sigma^2 (dB)^2.
\]
While \( a^2 (dt)^2 \) and \( 2a\sigma dB dt \) are non linear with respect to \( dt \) and \( dX \), the framed term turns out to be exactly \( \sigma^2 dt \).

Formally, this is a consequence of the basic formula\(^{47}\) \( dN \sim \sqrt{dt}N(0,1) \) that assigns \( \sqrt{dt} \) for the standard deviation of \( dB \).

Thus the differential of \( F \) along the trajectories of (2.147) is given by the following \textbf{Itô formula}:
\[
dF = \left\{ F_t + aF_x + \frac{1}{2} \sigma^2 F_{xx} \right\} dt + \sigma F_x dB. \tag{2.148}
\]
We are now ready to solve (2.146), that we write in the form
\[
dS = \mu S dt + \sigma S dB.
\]
Let \( F(S) = \log S \). Since
\[
F_t = 0, \quad F_S = \frac{1}{S}, \quad F_{SS} = -\frac{1}{S^2}
\]
\(^{47}\) See (2.86), subsection 2.4.3.
Itô’s formula gives, with $X = S$, $a(S, t) = \mu S$, $\sigma(S, t) = \sigma S$,

$$d \log S = \left( \mu - \frac{1}{2} \sigma^2 \right) dt + \sigma dB.$$ 

We can now integrate between $0$ and $t$, obtaining

$$\log S(t) = \log S_0 + \left( \mu - \frac{1}{2} \sigma^2 \right) t + \sigma B(t). \tag{2.149}$$

The (2.149) shows that the random variable $Y = \log S$ has a normal distribution, with mean $\log S_0 + \left( \mu - \frac{1}{2} \sigma^2 \right) t$ and variance $\sigma^2 t$. Its probability density is therefore

$$f(y) = \frac{1}{\sqrt{2\pi \sigma^2 t}} \exp \left\{ - \frac{(y - \log S_0 - \left( \mu - \frac{1}{2} \sigma^2 \right) t)^2}{2\sigma^2 t} \right\}.$$ 

and the density of $S$ is given by

$$p(s) = \frac{1}{s} f(\log s) = \frac{1}{s \sqrt{2\pi \sigma^2 t}} \left\{ - \frac{(\log s - \log S_0 - \left( \mu - \frac{1}{2} \sigma^2 \right) t)^2}{2\sigma^2 t} \right\}$$

which is called a lognormal density.

### 2.9.3 The Black-Scholes equation

We now construct a differential equation able to describe the evolution of $V(S, t)$. We work under the following hypotheses:

- $S$ follows a lognormal law.
- The volatility $\sigma$ is constant and known.
- There are no transaction costs or dividends.
- It is possible to buy or sell any number of the underlying asset.
- There is an interest rate $r > 0$, for a riskless investment. This means that 1 dollar in a bank at time $t = 0$ becomes $e^{rt}$ dollars at time $T$.
- The market is arbitrage free.

The last hypothesis is crucial in the construction of the model and means that there is no opportunity for instantaneous risk-free profit. It could be considered as a sort of conservation law for money!

The translation of this principle into mathematical terms is linked with the notion of hedging and the existence of self-financing portfolios\(^{48}\). The basic idea is first to compute the return of $V$ through Itô formula and then to construct a riskless portfolio $\Pi$, consisting of shares of $S$ and the option. By the arbitrage free hypothesis, $\Pi$ must grow at the current interest rate $r$, i.e. $d\Pi = r \Pi dt$, which turns out to coincide with the fundamental Black-Scholes equation.

\(^{48}\) A portfolio is a collection of securities (e.g. stocks) holdings.
Let us then use the Itô formula to compute the differential of $V$. Since 

$$dS = \mu Sdt + \sigma SdB,$$

we find 

$$dV = \left\{ V_t + \mu SV_S + \frac{1}{2} \sigma^2 S^2 V_{SS} \right\} dt + \sigma SV_S dB. \quad (2.150)$$

Now we try to get rid of the risk term $\sigma SV_S dB$ by constructing a portfolio $\Pi$, consisting of the option and a quantity $\Delta$ of underlying:

$$\Pi = V - S\Delta.$$

This is an important financial operation called hedging. Consider now the interval of time $(t, t + dt)$ during which $\Pi$ undergoes a variation $d\Pi$. If we manage to keep $\Delta$ equal to its value at $t$ during the interval $(t, t + dt)$, the variation of $\Pi$ is given by 

$$d\Pi = dV - \Delta dS.$$

This is a key point in the whole construction, that needs to be carefully justified\(^{49}\). Although we content ourselves with an intuitive level, we will come back to this question in the last section of this chapter.

Using (2.150) we find 

$$d\Pi = dV - \Delta dS = 
\left\{ V_t + \mu SV_S + \frac{1}{2} \sigma^2 S^2 V_{SS} - \mu S\Delta \right\} dt + \sigma S(V_S - \Delta) dB. \quad (2.151)$$

Thus, if we choose 

$$\Delta = V_S, \quad (2.152)$$

meaning that $\Delta$ is the value of $V_S$ at $t$, we eliminate the stochastic component in (2.151). The evolution of the portfolio $\Pi$ is now entirely deterministic and its dynamics is given by the following equation:

$$d\Pi = \left\{ V_t + \frac{1}{2} \sigma^2 S^2 V_{SS} \right\} dt. \quad (2.153)$$

The choice (2.152) appears almost .... miraculous, but it is partly justified by the fact that $V$ and $S$ are dependent and the random component in their dynamics is proportional to $S$. Thus, in a suitable linear combination of $V$ and $S$ such component should disappear.

It is the moment to use the no-arbitrage principle. Investing $\Pi$ at the riskless rate $r$, after a time $dt$ we have an increment $r\Pi dt$. Compare $r\Pi dt$ with $d\Pi$ given by (2.153).

\(^{49}\) We borrow from finance the use of the greek letter $\Delta$ in this context. Clearly here it has nothing to do with the Laplace operator.

\(^{50}\) In fact, saying that we keep $\Delta$ constant for an infinitesimal time interval so that we can cancel $Sd\Delta$ from the differential $d\Pi$ requires a certain amount of impudence....
\[ \text{If } d\Pi > r\Pi dt, \text{ we borrow an amount } \Pi \text{ to invest in the portfolio. The return } d\Pi \text{ would be greater of the cost } r\Pi dt, \text{ so that we make an instantaneous riskless profit } d\Pi - r\Pi dt. \]

\[ \text{If } d\Pi < r\Pi dt, \text{ we sell the portfolio } \Pi \text{ investing it in a bank at the rate } r. \text{ This time we would make an instantaneous risk free profit } r\Pi dt - d\Pi. \]

Therefore, the arbitrage free hypothesis forces

\[ d\Pi = \left\{ V_t + \frac{1}{2} \sigma^2 S^2 V_{SS} \right\} dt = r\Pi dt. \tag{2.154} \]

Substituting

\[ \Pi = V - S\Delta = V - V_S S \]

into (2.154), we obtain the celebrated **Black-Scholes equation**: \[ \mathcal{L}V = V_t + \frac{1}{2} \sigma^2 S^2 V_{SS} + rSV_S - rV = 0. \tag{2.155} \]

Note that the coefficient \( \mu \), the drift of \( S \), does not appear in (2.155). This fact is apparently counter-intuitive and shows an interesting aspect of the model. The financial meaning of the Black-Scholes equation is emphasized from the following decomposition of its right hand side:

\[ \mathcal{L}V = V_t + \frac{1}{2} \sigma^2 S^2 V_{SS} - r(V - SV_S). \]

The Black-Scholes equation is a little more general than the equations we have seen so far. Indeed, the diffusion and the drift coefficients are both depending on \( S \). However, as we shall see below, we can transform it into the diffusion equation \( u_t = u_{xx} \).

Observe that the coefficient of \( V_{SS} \) is positive, so that (2.155) is a **backward equation**. To get a well posed problem, we need a **final condition** (at \( t = T \)), a side condition at \( S = 0 \) and one condition for \( S \to +\infty \).

- **Final conditions**. We examine what conditions we have to impose at \( t = T \).

  - **Call**. If at time \( T \) we have \( S > E \) then we exercise the option, with a profit \( S - E \). If \( S \leq E \), we do not exercise the option with no profit. The **final payoff** of the option is therefore

    \[ C(S,T) = \max \{ S - E, 0 \} = (S - E)^+, \quad S > 0. \]

  - **Put**. If at time \( T \) we have \( S \geq E \), we do not exercise the option, while we exercise the option if \( S < E \). The **final payoff** of the option is therefore

    \[ P(S,T) = \max \{ E - S, 0 \} = (E - S)^+, \quad S > 0. \]
• Boundary conditions. We now examine the conditions to be imposed at $S = 0$ and for $S \to +\infty$.

Call. If $S = 0$ at a time $t$, (2.146) implies $S = 0$ thereafter, and the option has no value; therefore

$$C(0, t) = 0 \quad t \geq 0.$$  

As $S \to +\infty$, at time $t$, the option will be exercised and its value becomes practically equal to $S$ minus the discounted exercise price, that is

$$C(S, t) - (S - e^{-r(T-t)}E) \to 0 \quad \text{as } S \to \infty.$$  

Put. If at a certain time is $S = 0$, so that $S = 0$ thereafter, the final profit is $E$. Thus, to determine $P(0, t)$ we need to determine the present value of $E$ at time $T$, that is

$$P(0, t) = Ee^{-r(T-t)}.$$  

If $S \to +\infty$, we do not exercise the option, hence

$$P(S, t) = 0 \quad \text{as } S \to +\infty.$$  

2.9.4 The solutions

Let us summarize our model in the two cases.

**Black-Scholes equation**

$$V_t + \frac{1}{2} \sigma^2 S^2 V_{SS} + rSV_S - rV = 0. \quad (2.156)$$

**Final payoffs**

$$C(S, T) = (S - E)^+ \quad \text{(call)}$$

$$P(S, T) = (E - S)^+ \quad \text{(put).}$$

**Boundary conditions**

$$C(0, t) = 0, \quad C(S, t) - (S - e^{-r(T-t)}E) \to 0 \quad \text{as } S \to \infty \quad \text{(call)}$$

$$P(0, t) = Ee^{-r(T-t)}, \quad P(S, T) = 0 \quad \text{as } S \to \infty \quad \text{(put).}$$

It turns out that the above problems can be reduced to a global Cauchy problem for the heat equation. In this way it is possible to find explicit formulas for the solutions. First of all we make a change of variables to reduce the Black-Scholes equation to constant coefficients and to pass from backward to forward in time. Also note that $1/\sigma^2$ can be considered an intrinsic reference time while the exercise price $E$ gives a characteristic order of magnitude for $S$ and $V$. Thus, $1/\sigma^2$ and $E$ can be used as rescaling factors to introduce dimensionless variables.

Let us set

$$x = \log \frac{S}{E}, \quad \tau = \frac{1}{2} \sigma^2 (T - t), \quad w(x, \tau) = \frac{1}{E} V \left( Ee^x, T - \frac{2\tau}{\sigma^2} \right).$$
When $S$ goes from 0 to $+\infty$, $x$ varies from $-\infty$ to $+\infty$. When $t = T$ we have $\tau = 0$. Moreover:

$$V_t = -\frac{1}{2}\sigma^2 E w_\tau,$$

$$V_S = \frac{E}{S} w_x, \quad V_{SS} = -\frac{E}{S^2} w_x + \frac{E}{S^2} w_{xx}.$$ 

Substituting into (2.156), after some simplifications, we get

$$-\frac{1}{2}\sigma^2 w_\tau + \frac{1}{2}\sigma^2 (-w_x + w_{xx}) + rw_x - rw = 0$$

or

$$w_\tau = w_{xx} + (k - 1) w_x - kw$$

where $k = \frac{2r}{\sigma^2}$ is a dimensionless parameter. By further setting\(^{51}\)

$$w(x, \tau) = e^{-\frac{k-1}{2}x - \frac{(k+1)^2}{4} \tau} v(x, \tau)$$

we find that $v$ satisfies

$$v_\tau - v_{xx} = 0, \quad -\infty < x < +\infty, \ 0 \leq \tau \leq T.$$

The final condition for $V$ becomes an initial condition for $v$. Precisely, after some manipulations, we have

$$v(x, 0) = g(x) = \begin{cases} e^{\frac{1}{2}(k+1)x} - e^{\frac{1}{2}(k-1)x} & x > 0 \\ 0 & x \leq 0 \end{cases}$$

for the call option, and

$$v(x, 0) = g(x) = \begin{cases} e^{\frac{1}{2}(k-1)x} - e^{\frac{1}{2}(k+1)x} & x < 0 \\ 0 & x \geq 0 \end{cases}$$

for the put option.

Now we can use the preceding theory and in particular Theorem 2.3 and Corollary 2.3. The solution is unique and it is given by formula

$$v(x, \tau) = \frac{1}{\sqrt{4\pi \tau}} \int_R g(y) e^{-\frac{(y-x)^2}{4\tau}} dy.$$ 

To have a more significant formula, let $y = \sqrt{2\tau z} + x$; then, focusing on the call option:

$$v(x, \tau) = \frac{1}{\sqrt{2\pi}} \int_R g \left( \sqrt{2\tau z} + x \right) e^{-\frac{z^2}{2}} dy =$$

$$= \frac{1}{\sqrt{2\pi}} \left\{ \int_{-\infty}^{\infty} e^{\frac{1}{2}(k+1)(\sqrt{2\tau z} + x) - \frac{1}{2} z^2} dz - \int_{-\infty}^{\infty} e^{\frac{1}{2}(k-1)(\sqrt{2\tau z} + x) - \frac{1}{2} z^2} dz \right\}.$$

\(^{51}\) See Problem 2.14.
After some manipulations in the two integrals\textsuperscript{52}, we obtain
\[ v(x, \tau) = e^{1/2(x+1)^2 + 1/(k+1)^2 \tau} N(d_+) - e^{1/2(x-1)^2 + 1/(k-1)^2 \tau} N(d_-) \]
where
\[ N(z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{z} e^{-1/2 y^2} dy \]
is the distribution of a standard normal random variable and
\[ d_\pm = \frac{x}{\sqrt{2\tau}} + \frac{1}{2} (k \pm 1) \sqrt{2\tau}. \]

Going back to the original variables we have, for the call:
\[ C(S, t) = SN(d_+) - Ee^{-r(T-t)}N(d_-) \]

with
\[ d_\pm = \frac{\log(S/E) + (r \pm 1/2 \sigma^2)(T-t)}{\sigma \sqrt{T-t}}. \]

The formula for the put is
\[ P(S, t) = Ee^{-r(T-t)}N(-d_-) - SN(-d_+). \]

It can be shown that\textsuperscript{53}
\[ \Delta = C_S = N(d_+) > 0 \quad \text{for the call} \]
\[ \Delta = P_S = N(d_+) - 1 < 0 \quad \text{for the put.} \]

Note that \( C_S \) and \( P_S \) are strictly increasing with respect to \( S \), since \( N \) is a strictly increasing function and \( d_+ \) is strictly increasing with \( S \). The functions \( C, P \) are therefore \textit{strictly convex functions} of \( S \), for every \( t \), namely \( C_{SS} > 0 \) and \( P_{SS} > 0 \).

- \textit{Put-call parity}. Put and call options with the same exercise price and expiry time can be connected by forming the following portfolio:
\[ \Pi = S + P - C \]

\textsuperscript{52} For instance, to evaluate the first integral, complete the square at the exponent, writing
\[ \frac{1}{2} (k + 1) \left( \sqrt{2\tau} z + x \right) - \frac{1}{2} z^2 = \frac{1}{2} (k + 1) x + \frac{1}{4} (k + 1)^2 \tau - \frac{1}{2} \left[ z - \frac{1}{2} (k + 1) \sqrt{2\tau} \right]^2. \]

Then, setting \( y = \frac{1}{2} (k + 1) \sqrt{2\tau} \),
\[ \int_{-x/\sqrt{2\tau}}^{\infty} e^{1/2(k+1)(\sqrt{2\tau} z + x) - 1/2 z^2} dz = e^{1/4(k-1)^2 \tau} \int_{-x/\sqrt{2\tau} - (k+1) \sqrt{\tau}/\sqrt{2}}^{\infty} e^{-1/2 y^2} dy. \]

\textsuperscript{53} The calculations are rather ... painful.
where the minus in front of $C$ shows a so called short position (negative holding). For this portfolio the final payoff is

$$
\Pi (S,T) = S + (E - S)^+ - (S - E)^+.
$$

If $E \geq S$, we have

$$
\Pi (S,T) = S + (E - S) - 0 = E
$$

while if $E \leq S$,

$$
\Pi (S,T) = S + 0 - (S - E) = E.
$$

Thus at expiry the payoff is always equal to $E$ and it constitutes a riskless profit, whose value at $t$ must be equal to the discounted value of $E$, because of the no arbitrage condition. Hence we find the following relation (put-call parity)

$$
S + P - C = E e^{-r(T-t)}.
$$

(2.157)

Formula (2.157) also shows that, given the value of $C$ (or $P$), we can find the value of $P$ (or $C$).

From (2.157), since $E e^{-r(T-t)} \leq E$ and $P \geq 0$, we get

$$
C (S,t) = S + P - E e^{-r(T-t)} \geq S - E
$$

and therefore, since $C \geq 0$,

$$
C (S,t) \geq (S - E)^+.
$$

It follows that the value of $C$ is always greater than the final payoff. It is not so for a put. In fact

$$
P (0,t) = E e^{-r(T-t)} \leq E
$$

so that the value of $P$ is below the final payoff when $S$ is near 0, while it is above just before expiring. The figures 2.14 and 2.15 show the behavior of $C$ and $P$ versus $S$, for some values of $T - t$ up to expiry.

Fig. 2.14. The value function for an European call option
Fig. 2.15. The value function of an European put option

- **Different volatilities.** The maximum principle arguments in subsection 2.8.3 can be used to compare the value of two options with different volatilities $\sigma_1$ and $\sigma_2$, having the same exercise price $E$ and the same strike time $T$. Assume that $\sigma_1 > \sigma_2$ and denote by $C^{(1)}$, $C^{(2)}$ the value of the corresponding call options. Diminishing the amount of risk the value of the option should decrease and indeed we want to confirm that

$$C^{(1)} > C^{(2)} \quad S > 0, 0 \leq t < T.$$ 

Let $W = C^{(1)} - C^{(2)}$. Then

$$W_t + \frac{1}{2} \sigma_2^2 S^2 W_{SS} + rSW_S - rW = \frac{1}{2} (\sigma_2^2 - \sigma_1^2) S^2 C^{(1)}_{SS}$$  \hspace{1cm} (2.158)$$

with $W(S,T) = 0$, $W(0,t) = 0$ and $W \to 0$ as $S \to +\infty$.

The (2.158) is a nonhomogeneous equation, whose right hand side is negative for $S > 0$, because $C^{(1)}_{SS} > 0$. Since $W$ is continuous in the half strip $[0, +\infty) \times [0, T]$ and vanishes at infinity, it attains its global minimum at a point $(S_0, t_0)$.

We claim that the minimum is zero and cannot be attained at a point in $(0, +\infty) \times [0, T)$. Since the equation is backward, $t_0 = 0$ is excluded. Suppose $W(S_0, t_0) \leq 0$ with $S_0 > 0$ and $0 < t_0 < T$. We have

$$W_t(S_0, t_0) = 0$$

and

$$W_S(S_0, t_0) = 0, \quad W_{SS}(S_0, t_0) \geq 0.$$ 

Substituting $S = S_0, t = t_0$ into (2.158) we get a contradiction. Therefore $W = C^{(1)} - C^{(2)} > 0$ for $S > 0, 0 < t < T$. 
2.9.5 Hedging and self-financing strategy

The mathematical translation of the no arbitrage principle can be made more rigorously than we did in subsection 2.9.2, by introducing the concept of self-financing portfolio. The idea is to “duplicate” $V$ by means of a portfolio consisting of a number of shares of $S$ and a bond $Z$, a free risk investment growing at the rate $r$, e.g. $Z(t) = e^{rt}$.

To this purpose let us try to determine two processes $\phi = \phi(t)$ and $\psi = \psi(t)$ such that

$$V = \phi S + \psi Z \quad (0 \leq t \leq T) \quad (2.159)$$

in order to eliminate any risk factor. In fact, playing the part of the subscriber (that has to sell), the risk is that at time $T$ the price $S(T)$ is greater than $E$, so that the holder will exercise the option. If in the meantime the subscriber has constructed the portfolio (2.159), the profit from it exactly meets the funds necessary to pay the holder. On the other hand, if the option has zero value at time $T$, the portfolio has no value as well.

For the operation to make sense, it is necessary that the subscriber does not put extra money in this strategy (hedging). This can be assured by requiring that the portfolio (2.159) be self-financing that is, its changes in value be dependent from variations of $S$ and $Z$ alone.

In formulas, this amount to requiring

$$dV = \phi dS + \psi dZ \quad (0 \leq t \leq T). \quad (2.160)$$

Actually, we have already met something like (2.160), when we have constructed the portfolio $\Pi = V - S\Delta$ or

$$V = \Pi + S\Delta,$$

asking that $dV = d\Pi + \Delta dS$. This construction is nothing else that a duplication of $V$ by means of a self-financing portfolio, with $\Pi$ playing the role of $Z$ and choosing $\psi = 1$.

But, what is the real meaning of (2.160)? We see it better in a discrete setting. Consider a sequence of times

$$t_0 < t_1 < ... < t_N$$

and suppose that the intervals $(t_j - t_{j-1})$ are very small. Denote by $S_j$ e $Z_j$ the values at $t_j$ of $S$ and $Z$. Consequently, look for two sequences

$$\phi_j \text{ and } \psi_j$$

corresponding to the quantity of $S$ and $Z$ to be used in the construction of the portfolio (2.159) from $t_{j-1}$ to $t_j$. Notice that $\phi_j$ and $\psi_j$ are chosen at time $t_{j-1}$.

Thus, given the interval $(t_{j-1}, t_j)$,

$$V_j = \phi_j S_j + \psi_j Z_j$$
represents the closing value of the portfolio while

\[ \phi_{j+1} S_j + \psi_{j+1} Z_j \]

is the opening value, the amount of money necessary to buy the new one. The **self-financing condition means** that the value \( V_j \) of the portfolio at time \( t_j \), determined by the couple \((\phi_j, \psi_j)\), exactly meets the purchasing cost of the portfolio in the interval \((t_j, t_{j+1})\), determined by \((\phi_{j+1}, \psi_{j+1})\). This means

\[ \phi_{j+1} S_j + \psi_{j+1} Z_j = \phi_j S_j + \psi_j Z_j \quad (2.161) \]

or that **the financial gap**

\[ D_j = \phi_{j+1} S_j + \psi_{j+1} Z_j - V_j \]

**must be zero**, otherwise an amount of cash \( D_j \) has to be injected to substatin the strategy \((D_j > 0)\) or the same amount of money can be drawn from it \((D_j < 0)\). From (2.161) we deduce that

\[
V_{j+1} - V_j = (\phi_{j+1} S_{j+1} + \psi_{j+1} Z_{j+1}) - (\phi_j S_j + \psi_j Z_j) \\
= (\phi_{j+1} S_{j+1} + \psi_{j+1} Z_{j+1}) - (\phi_{j+1} S_j + \psi_{j+1} Z_j) \\
= \phi_{j+1} (S_{j+1} - S_j) + \psi_{j+1} (Z_{j+1} - Z_j)
\]

or

\[ \Delta V_j = \phi_{j+1} \Delta S_j + \psi_{j+1} \Delta Z_j \]

whose continuous version is exactly (2.160).

Going back to the continuous case, by combining formulas (2.150) and (2.160) for \( dV \), we get

\[
\left\{ V_t + \mu SV_S + \frac{1}{2} \sigma^2 S^2 V_{SS} \right\} dt + \sigma SV_S dB = \phi (\mu S dt + \sigma S dB) + \psi r Z dt.
\]

Choosing \( \phi = V_S \), we rediscover the Black and Scholes equation

\[
V_t + \frac{1}{2} \sigma^2 S^2 V_{SS} + r SV_S - r V = 0. \quad (2.162)
\]

On the other hand, if \( V \) satisfies (2.162) and

\[ \phi = V_S, \quad \psi = Z^{-1}(V - V_S S) = e^{-rt}(V - V_S S), \]

it can be proved that the self financing condition (2.160) is satisfied for the portfolio \( \phi S + \psi Z \).
2.10 Some Nonlinear Aspects

All the mathematical models we have examined so far are linear. On the other hand, the nature of most real problems is nonlinear. For example, nonlinear diffusion has to be taken into account in filtration problems, non linear drift terms are quite important in fluid dynamics while nonlinear reaction terms occur frequently in population dynamics and kinetics chemistry.

The presence of a nonlinearity in a mathematical model gives rise to many interesting phenomena that cannot occur in the linear case; typical instances are finite speed of diffusion, finite time blow-up or existence of travelling wave solutions of certain special profiles, each one with its own characteristic velocity.

In this section we try to convey some intuition of what could happen in two typical and important examples from filtration through a porous medium and population dynamics. In Chapter 4, we shall deal with nonlinear transport models.

2.10.1 Nonlinear diffusion. The porous medium equation

Consider a gas of density $\rho = \rho(x, t)$ flowing through a porous medium. Denote by $v = v(x, t)$ the velocity of the gas and by $\kappa$ the porosity of the medium, representing the volume fraction filled with gas. Conservation of mass reads, in this case:

$$\kappa \rho_t + \text{div} (\rho v) = 0. \quad (2.163)$$

Besides (2.163), the flow is governed by the two following constitutive (empirical) laws.

- **Darcy’s law:**
  $$v = -\frac{\mu}{\nu} \nabla p \quad (2.164)$$
  where $p = p(x, t)$ is the pressure, $\mu$ is the permeability of the medium and $\nu$ is the viscosity of the gas. We assume $\mu$ and $\nu$ are positive constants.

- **Equation of state:**
  $$p = p_0 \rho^\alpha \quad p_0 > 0, \alpha > 0. \quad (2.165)$$

From (2.164) and (2.165) we have, since $p^{1/\alpha} \nabla p = (1 + 1/\alpha)^{-1} \Delta (p^{1+1/\alpha})$,

$$\text{div} (\rho v) = -\frac{\mu}{(1 + 1/\alpha) \nu p_0^{1/\alpha}} \Delta (p^{1+1/\alpha}) = -\frac{(m - 1) \mu p_0}{m \nu} \Delta (\rho^m)$$

where $m = 1 + \alpha > 1$. From (2.163) we obtain

$$\rho_t = \frac{(m - 1) \mu p_0}{\kappa m \nu} \Delta (\rho^m).$$
Rescaling time \( t \mapsto \frac{(m - 1) \mu p_0}{k m \nu} t \) we finally get the **porous medium equation**

\[
\rho_t = \Delta(\rho^m). \tag{2.166}
\]

Since

\[
\Delta(\rho^m) = \text{div} \left( m \rho^{m-1} \nabla \rho \right)
\]

we see that the diffusion coefficient is \( D(\rho) = m \rho^{m-1} \), showing that the diffusive effect increases with the density.

The porous medium equation can be written in terms of the pressure variable

\[
u = \frac{p}{p_0} = \rho^{m-1}.
\]

It is not difficult to check that the equation for \( u \) is given by

\[
u_t = u \Delta u + \frac{m}{m - 1} |\nabla u|^2 \tag{2.167}
\]

showing once more the dependence on \( u \) of the diffusion coefficient.

One of the basic questions related to the equation (2.166) or (2.167) is to understand how an initial data \( \rho_0 \), confined in a small region \( \Omega \), evolves with time. The key object to examine is therefore the unknown boundary \( \partial \Omega \), or free boundary of the gas, whose speed of expansion we expect to be proportional to \( |\nabla u| \) (from (2.164)). This means that we expect a finite speed of propagation, in contrast with the classical case \( m = 1 \).

The porous media equation cannot be treated by elementary means, since at very low density the diffusion has a very low effect and the equation degenerates. However we can get some clue of what happens by examining a sort of fundamental solutions, the so called Barenblatt solutions, in spatial dimension 1.

The equation is

\[
\rho_t = (\rho^m)_{xx}. \tag{2.168}
\]

We look for **nonnegative self-similar** solutions of the form

\[
\rho(x, t) = t^{-\alpha} U(x t^{-\beta}) \equiv t^{-\alpha} U(\xi)
\]

satisfying

\[
\int_{-\infty}^{+\infty} \rho(x, t) \, dx = 1.
\]

This condition requires

\[
1 = \int_{-\infty}^{+\infty} t^{-\alpha} U(x t^{-\beta}) \, dx = t^{\beta - \alpha} \int_{-\infty}^{+\infty} U(\xi) \, d\xi
\]

so that we must have \( \alpha = \beta \) and \( \int_{-\infty}^{+\infty} U(\xi) \, d\xi = 1 \). Substituting into (2.168), we find

\[
\alpha t^{-\alpha - 1} (-U - \xi U') = t^{-m \alpha - 2\alpha} (U^m)''.
\]
Thus, if we choose $\alpha = 1/(m + 1)$, we get for $U$ the differential equation

$$(m + 1) (U^m)'' + \xi U' + U = 0$$

that can be written in the form

$$\frac{d}{d\xi} [(m + 1) (U^m)' + \xi U] = 0.$$ 

Thus, we have

$$(m + 1) (U^m)' + \xi U = \text{constant.}$$

Choosing the constant equal to zero, we get

$$(m + 1) (U^m)' = (m + 1) mU^{m-1}U' = -\xi U$$

or

$$(m + 1) mU^{m-2}U' = -\xi.$$ 

This in turn is equivalent to

$$\frac{(m + 1) m}{m - 1} (U^{m-1})' = -\xi$$

whose solution is

$$U (\xi) = [A - B_m \xi^2]^{1/(m-1)}$$

where $A$ is an arbitrary constant and $B_m = (m - 1) / 2m (m + 1)$. Clearly, to have a physical meaning, we must have $A > 0$ and $A - B_m \xi^2 \geq 0$.

In conclusion we have found solutions of the porous medium equation of the form

$$\rho(x, t) = \begin{cases} 
\frac{1}{t^\alpha} \left[ A - B_m \frac{x^2}{t^{2\alpha}} \right]^{1/(m-1)} & \text{if } x^2 \leq A t^{2\alpha} / B_m \\
0 & \text{if } x^2 > A t^{2\alpha} / B_m.
\end{cases} \quad (\alpha = 1/(m + 1)).$$

known as Barenblatt solutions. The points

$$x = \pm \sqrt{A/B_m} t^{\alpha} \equiv \pm r(t)$$

represent the gas interface between the part filled by gas and the empty part. Its speed of propagation is therefore

$$\dot{r} (t) = \alpha \sqrt{A/B_m} t^{\alpha - 1}.$$
Fig. 2.16. The Barenblatt solution
\[
\rho(x,t) = t^{-1/5} \left[ 1 - x^2 t^{-2/5} \right]^{1/3}
\]
for \( t = 1, 4, 10, 30 \)

2.10.2 Nonlinear reaction. Fischer’s equation

In 1937 Fisher\(^54\) introduced a model for the spatial spread of a so called favoured\(^55\) (or advantageous) gene in a population, over an infinitely long one dimensional habitat. Denoting by \( v \) the gene concentration, Fisher’s equation reads
\[
v_\tau = D v_{yy} + rv \left( 1 - \frac{v}{M} \right) \quad \tau > 0, \ y \in \mathbb{R}, \quad (2.169)
\]
where \( D, r, \) and \( M \) are positive parameters. An important question is to determine whether the gene has a typical speed of propagation.

Accordingly to the terminology in the introduction, (2.169) is a semilinear equation where diffusion is coupled with logistic growth through the reaction term
\[
f(v) = rv \left( 1 - \frac{v}{M} \right).
\]
The parameter \( r \) represents a biological potential (net birth-death rate, with dimension \([\text{time}]^{-1}\)), while \( M \) is the carrying capacity of the habitat. If we rescale time, space and concentration in the following way
\[
t = r\tau, \quad x = \sqrt{r/D} y, \quad u = v/M,
\]
(2.169) takes the dimensionless form
\[
 u_t = u_{xx} + u \left( 1 - u \right), \quad t > 0. \quad (2.170)
\]

Note the two equilibria \( u \equiv 0 \) and \( u \equiv 1 \). In absence of diffusion, 0 is unstable, and 1 is asymptotically stable. A trajectory with initial data \( u(0) = u_0 \) between 0 and 1 has the typical behavior shown in figure 2.17:


\(^{55}\) That is a gene that has an advantage in the struggle for life.
Fig. 2.17. Logistic curve $(r = 0.1, u_0 = 1/3)$

Therefore, if

$$u(x, 0) = u_0(x), \quad x \in \mathbb{R}, \quad (2.171)$$

is an initial data for the equation (2.169), with $0 < u_0(x) < 1$, we expect a competitive action between diffusion and reaction, with diffusion trying to spread and lower $u_0$ against the reaction tendency to increase $u$ towards the equilibrium solution 1.

What we intend to show here is the existence of permanent travelling waves solutions connecting the two equilibrium states, that is solutions of the form

$$u(x, t) = U(z), \quad z = x - ct,$$

with $c$ denoting the propagation speed, satisfying the conditions

$$0 < u < 1, \quad t > 0, x \in \mathbb{R}$$

and

$$\lim_{x \to -\infty} u(x, t) = 1 \quad \text{and} \quad \lim_{x \to +\infty} u(x, t) = 0. \quad (2.172)$$

The first condition in (2.172), states that the gene concentration is saturated at the far left end while the second condition denotes zero concentration at the far right end. Clearly, this kind of solutions realize a balance between diffusion and reaction.

Since the equation (2.169) is invariant under the transformation $x \mapsto -x$, it suffices to consider $c > 0$, that is right-moving waves only.

Since

$$u_t = -c U', \quad u_x = U', \quad u_{xx} = U'', \quad (' = d/dz)$$

substituting $u(x, t) = U(z)$ into (2.170), we find for $U$ the ordinary differential equation

$$U'' + c U' + U - U^2 = 0 \quad (2.173)$$
with
\[ \lim_{z \to -\infty} U(z) = 1 \quad \text{and} \quad \lim_{z \to +\infty} U(z) = 0. \] (2.174)

Letting \( U' = V \), the equation (2.173) is equivalent to the system
\[
\frac{dU}{dz} = V, \quad \frac{dV}{dz} = -cV - U + U^2
\] (2.175)
in the phase plane \((U, V)\). This system has two equilibrium points \((0, 0)\) and \((1, 0)\) corresponding to two steady states. Our travelling wave solution corresponds to an orbit connecting \((1, 0)\) to \((0, 0)\), with \(0 < U < 1\).

We first examine the local behavior of the orbits near the equilibrium points. The coefficients matrices of the linearized systems at \((0, 0)\) and \((1, 0)\) are, respectively,
\[
J(0, 0) = \begin{pmatrix} 0 & 1 \\ -1 & -c \end{pmatrix} \quad \text{and} \quad J(1, 0) = \begin{pmatrix} 0 & 1 \\ 1 & -c \end{pmatrix}.
\]
The eigenvalues of \(J(0, 0)\) are
\[ \lambda_\pm = \frac{1}{2} \left[ -c \pm \sqrt{c^2 - 4} \right], \]
with corresponding eigenvectors
\[ h_\pm = \begin{pmatrix} -c \pm \sqrt{c^2 - 4} \\ 2 \end{pmatrix}. \]
If \(c \geq 2\) the eigenvalues are both negative while if \(c < 2\) they are complex. Therefore \((0, 0)\) is a \( \left\{ \begin{array}{ll} \text{stable node} & \text{if } c \geq 2 \\ \text{stable focus} & \text{if } c < 2 \end{array} \right. \)

The eigenvalues of \(J(1, 0)\) are
\[ \mu_\pm = \frac{1}{2} \left[ -c \pm \sqrt{c^2 + 4} \right], \]
of opposite sign, hence \((1, 0)\) is a saddle point. The unstable and stable separatrices leave \((1, 0)\) along the directions of the two eigenvectors
\[ k_+ = \begin{pmatrix} c + \sqrt{c^2 + 4} \\ 2 \end{pmatrix} \quad \text{and} \quad k_- = \begin{pmatrix} c - \sqrt{c^2 + 4} \\ 2 \end{pmatrix}, \]
respectively.

Now, the constraint \(0 < U < 1\) rules out the case \(c < 2\), since in this case \(U\) changes sign along the orbit approaching \((0, 0)\). For \(c \geq 2\), all orbits\(^{56}\) in a neighborhood of the origin approach \((0, 0)\) for \(z \to +\infty\) asymptotically with slope

\(^{56}\) Except for two orbits on the stable manifold tangent to \(h_-\) at \((0, 0)\), in the case \(c > 2\)
\( \lambda_+ \). On the other hand, the only orbit going to \((1, 0)\) as \(z \to -\infty\) and remaining in the region \(0 < U < 1\) is the unstable separatrix \(\gamma\) of the saddle point.

Figure 2.18 shows the orbits configuration in the region of interest (see Problem 2.23). The conclusion is that for each \(c \geq 2\) there exists a unique travelling wave solution of equation (2.169) with speed \(c\). Moreover \(U\) is strictly decreasing.

In terms of original variables, there is a unique travelling wave solution for every speed \(c\) satisfying the inequality \(c \geq c_{\text{min}} = 2\sqrt{rD}\).

Thus, we have a continuous “spectrum” of possible speeds of propagation. It turns out that the minimum speed \(c = c_{\text{min}}\) is particularly important.

Indeed, having found a travelling solution is only the beginning of the story. There is a number of questions that arise naturally. Among them, the study of the stability of the travelling waves or of the asymptotic behavior (as \(t \to +\infty\)) of a solution with an initial data \(u_0\) of transitional type, that is

\[
 u_0(x) = \begin{cases} 
 1 & x \leq a \\
 0 & a < x < b \\
 0 & x \geq b.
\end{cases}
\]  

(2.176)

Should we expect that the travelling wave is insensitive to small perturbations? Does the solution with initial condition (2.176) evolve towards one of the travelling waves we have just found?

The interested reader can find the answers in the many specialized texts or papers on the subject\(^{57}\). Here we only mention that among the travelling wave solutions we have found, only the minimum speed one can be the asymptotic representation of solutions with transitional type initial condition. The biological implication of this result is that \(c_{\text{min}}\) determines the required speed of propagation of an advantageous gene.

---

\(^{57}\) See for instance, the books by Murray, vol I, 2001, or Grindrod, 1991.
Problems

2.1. Use the method of separation of variables to solve the following initial-Neumann problem:

\[
\begin{align*}
&u_t - u_{xx} = 0 \quad 0 < x < L, \ t > 0 \\
&u(x,0) = x \quad 0 < x < L \\
&u_x(0,t) = u_x(L,t) = 0 \quad t > 0.
\end{align*}
\]

2.2. Use the method of separation of variables to solve the following nonhomogeneous initial-Neumann problem:

\[
\begin{align*}
&u_t - u_{xx} = tx \quad 0 < x < \pi, \ t > 0 \\
&u(x,0) = 1 \quad 0 \leq x \leq \pi \\
&u_x(0,t) = u_x(L,t) = 0 \quad t > 0.
\end{align*}
\]

[Hint: Write the candidate solution as \( u(x,t) = \sum_{k \geq 0} c_k(t) v_k(x) \) where \( v_k \) are the eigenfunctions of the eigenvalue problem associated with the homogeneous equation.]

2.3. Use the method of separation of variables to solve (at least formally) the following mixed problem:

\[
\begin{align*}
&u_t - Du_{xx} = 0 \quad 0 < x < \pi, \ t > 0 \\
&u(x,0) = g(x) \quad 0 \leq x \leq \pi \\
&u_x(0,t) = 0 \\
&u_x(L,t) + u(L,t) = U \quad t > 0.
\end{align*}
\]

[Answer: \( u(x,t) = \sum_{k \geq 0} c_k e^{-D\mu_k^2 t} \cos \mu_k x \), where the numbers \( \mu_k \) are the positive solutions of the equation \( \tan \mu = 1 \).]

2.4. Prove that, if \( w_t - D\Delta w = 0 \) in \( Q_T \) and \( w \in C(\overline{Q_T}) \), then

\[
\min_{\partial_p Q_T} w \leq w(x,t) \leq \max_{\partial_p Q_T} w \quad \text{for every } (x,t) \in Q_T.
\]

2.5. Prove Corollary 2.1.

[Hint: b). Let \( u = v - w, \ M = \max_{\overline{Q_T}} |f_1 - f_2| \) and apply Theorem 2.2 to \( z_\pm = \pm u - Mt \).]

2.6. Let \( g(t) = M \) for \( 0 \leq t \leq 1 \) and \( g(t) = M - (1 - t)^4 \) for \( 1 < t \leq 2 \). Let \( u \) be the solution of \( u_t - u_{xx} = 0 \) in \( Q_2 = (0,2) \times (0,2), \ u = g \) on \( \partial_p Q_2 \). Compute \( u(1,1) \) and check that it is the maximum of \( u \). Is this in contrast with the strong maximum principle of Remark 2.4?

2.7. Suppose \( u = u(x,t) \) is a solution of the heat equation in a plane domain \( D_T = Q_T \setminus (\overline{Q_1} \cup \overline{Q_2}) \) where \( Q_1 \) and \( Q_2 \) are the rectangles in figure 2.19. Assume that \( u \) attains its maximum \( M \) at the interior point \( (x_1,t_1) \). Where else \( u = M \)?
2.9. Determine for which \( \alpha \) and \( \beta \) there exist similarity solutions to \( u_t - u_{xx} = f(x) \) of the form \( t^\alpha U(x/t^\beta) \) in each one of the following cases:

(a) \( f(x) = 0 \),  
(b) \( f(x) = 1 \),  
(c) \( f(x) = x \).

[Answer: (a) \( \alpha \) arbitrary, \( \beta = 1/2 \).  
(b) \( \alpha = 1 \), \( \beta = 1/2 \).  
(c) \( \alpha = 3/2 \), \( \beta = 1/2 \)].

2.10. (Reflecting barriers and Neumann condition). Consider the symmetric random walk of Section 2.4. Suppose that a perfectly reflecting barrier is located at the point \( L = \overline{m}h + \frac{h}{2} > 0 \). By this we mean that if the particle hits the point \( L - \frac{h}{2} \) at time \( t \) and moves to the right, then it is reflected and it comes back to \( L - \frac{h}{2} \) at time \( t + \tau \). Show that when \( h, \tau \to 0 \) and \( h^2/\tau = 2D \), \( p = p(x,t) \) is a solution of the problem

\[
\begin{cases}
p_t - Dp_{xx} = 0 & x < L, t > 0 \\
p(x,0) = \delta & x < L \\
p_x(L,t) = 0 & t > 0
\end{cases}
\]

and moreover \( \int_{-\infty}^{L} p(x,t) \, dx = 1 \). Compute explicitly the solution.

[Answer: \( p(x,t) = \Gamma_D(x,t) + \Gamma_D(x-2L,t) \)].

2.11. (Absorbing barriers and Dirichlet condition). Consider the symmetric random walk of Section 2.4. Suppose that a perfectly absorbing barrier is located at the point \( L = \overline{m}h > 0 \). By this we mean that if the particle hits the point \( L - h \)
at time $t$ and moves to the right then it is absorbed and stops at $L$. Show that when $h, \tau \to 0$ and $h^2/\tau = 2D$, $p = p(x,t)$ is a solution of the problem

\[
\begin{cases}
p_t - Dp_{xx} = 0 & x < L, t > 0 \\
p(x,0) = \delta & x < L \\
p(L,t) = 0 & t > 0
\end{cases}
\]

Compute explicitly the solution.

[Answer: $p(x,t) = \Gamma_D(x,t) - \Gamma_D(x-2L,t)$]

2.12. Use the partial Fourier transform $\hat{u}(\xi, t) = \int_{\mathbb{R}} e^{-ix\xi} u(x,t) \, dx$ to solve the global Cauchy problem (2.129) and rediscover formula (2.130).

2.13. Prove Theorem 2.5 under the condition $z(x,t) \leq C$, $x \in \mathbb{R}$, $0 \leq t \leq T$ , using the following steps.

a) Let $\sup_{\mathbb{R}} z(x,0) = M_0$ and define

$$w(x,t) = \frac{2C}{L^2} (\frac{x^2}{2} + Dt) + M_0.$$ 

Check that $w_t - Dw_{xx} = 0$ and use the maximum principle to show that $w \geq z$ in the rectangle $R_L = [-L, L] \times [0, T]$.

b) Fix an arbitrary point $(x_0, t_0)$ and choose $L$ large enough to have $(x_0, t_0) \in R_L$. Using a) deduce that $z(x_0, t_0) \leq M_0$.

2.14. Find an explicit formula for the solution of the global Cauchy problem

\[
\begin{cases}
  u_t = Du_{xx} + bu_x + cu & x \in \mathbb{R}, t > 0 \\
  u(x,0) = g(x) & x \in \mathbb{R}.
\end{cases}
\]

where $D, b, c$ are constant coefficients. Show that, if $c < 0$ and $g$ is bounded, $u(x,t) \to 0$ as $t \to +\infty$.

[Hint: Choose $h, k$ such that $v(x,t) = u(x,t)e^{hx+kt}$ is a solution of $v_t = Dv_{xx}$].

2.15. Find an explicit formula for the solution of the Cauchy problem

\[
\begin{cases}
  u_t = u_{xx} & x > 0, t > 0 \\
  u(x,0) = g(x) & x \geq 0 \\
  u(0,t) = 0 & t > 0.
\end{cases}
\]

with $g$ continuous and $g(0) = 0$.

[Hint: Extend $g$ to $x < 0$ by odd reflection: $g(-x) = -g(x)$. Solve the corresponding global Cauchy problem and write the result as an integral on $(0, +\infty)$].

2.16. Let $Q_T = \Omega \times (0, T)$, with $\Omega$ bounded domain in $\mathbb{R}^n$. Let $u \in C^{2,1}(Q_T) \cap C(\overline{Q_T})$ satisfy the equation

$$u_t = D\Delta u + b(x,t) \cdot \nabla u + c(x,t) u$$

in $Q_T$. 

where \( b \) and \( c \) are continuous in \( \overline{Q}_T \). Show that if \( u \geq 0 \) (resp. \( u \leq 0 \)) on \( \partial \rho Q_T \) then \( u \geq 0 \) (resp. \( u \leq 0 \)) in \( Q_T \).

**[Hint: Assume first that \( c(x,t) \leq a < 0 \). Then reduce to this case by setting \( u = ve^{kt} \) with a suitable \( k > 0 \).]**

2.17. Fill in the details in the arguments of Section 6.2, leading to formulas (2.108) and (2.109).

2.18. Solve the following initial-Dirichlet problem in \( B_1 = \{ x \in \mathbb{R}^3 : |x| < 1 \} \):

\[
\begin{cases}
  u_t = \Delta u & x \in B_1, t > 0 \\
  u(x,0) = 0 & x \in B_1 \\
  u(\sigma,t) = 1 & \sigma \in \partial B_1, t > 0.
\end{cases}
\]

Compute \( \lim_{t \to +\infty} u \).

**[Hint: The solution is radial so that \( u = u(r,t), r = |x| \). Observe that \( \Delta u = u_{rr} + \frac{2}{r} u_r = \frac{1}{r} (ru)_{rr} \). Let \( v = ru \), reduce to homogeneous Dirichlet condition and use separation of variables].**

2.19. Solve the following initial-Dirichlet problem

\[
\begin{cases}
  u_t = \Delta u & x \in K, t > 0 \\
  u(x,0) = |x| & x \in K \\
  u(\sigma,t) = 1 & \sigma \in \partial K, t > 0.
\end{cases}
\]

where \( K \) is the rectangular box

\( K = \{ (x,y,z) \in \mathbb{R}^3 : 0 < x < a, 0 < y < b, 0 < z < c \} \).

Compute \( \lim_{t \to +\infty} u \).

2.20. Solve the following initial-Neumann problem in \( B_1 = \{ x \in \mathbb{R}^3 : |x| < 1 \} \):

\[
\begin{cases}
  u_t = \Delta u & x \in B_1, t > 0 \\
  u(x,0) = |x| & x \in B_1 \\
  u(\nu,\sigma,t) = 1 & \sigma \in \partial B_1, t > 0.
\end{cases}
\]

2.21. Solve the following non homogeneous initial-Dirichlet problem in the unit sphere \( B_1 (u = u(r,t), r = |x|) \):

\[
\begin{cases}
  u_t - (u_{rr} + \frac{2}{r} u_r) = q e^{-t} & 0 < r < 1, t > 0 \\
  u(r,0) = U & 0 \leq r \leq 1 \\
  u(1,t) = 0 & t > 0.
\end{cases}
\]

**[Answer: The solution is]

\[
u(r,t) = \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^n}{\lambda_n} \sin(\lambda_n r) \left\{ \frac{q}{1 - \lambda_n^2} \left( e^{-t} - e^{-\lambda_n^2 t} \right) - U e^{-\lambda_n^2 t} \right\}
\]

where \( \lambda_n = n\pi \).
2.22. Using the maximum principle, compare the values of two call options \( C^{(1)} \) and \( C^{(2)} \) in the following cases:

(a) Same exercise price and \( T_1 > T_2 \). (b) Same expiry time and \( E_1 > E_2 \).

2.23. Justify carefully the orbit configuration of figure 2.18 and in particular that the unstable orbit \( \gamma \) connects the two equilibrium points of system (2.175), by filling in the details in the following steps:

1. Let \( \mathbf{F} = \mathbf{V} + (\mathbf{U} - \mathbf{U}^2 - \mathbf{U}) \mathbf{j} \) and \( \mathbf{n} \) be the interior normal to the boundary of the triangle \( \Omega \) in figure 2.20. Show that, if \( \beta \) is large enough, \( \mathbf{F} \cdot \mathbf{n} > 0 \) along \( \partial \Omega \).

2. Deduce that all the orbits of system (2.175) starting at a point in \( \Omega \) cannot leave \( \Omega \) (i.e. \( \Omega \) is a \textit{positively invariant region}) and converge to the origin as \( z \to +\infty \).

3. Finally, deduce that the unstable separatrix \( \gamma \) of the saddle point \((1, 0)\) approaches \((0, 0)\) as \( z \to +\infty \).

![Fig. 2.20. Trapping region for the orbits of the vector field \( \mathbf{F} = \mathbf{V} + (\mathbf{U} - \mathbf{U}^2 - \mathbf{U}) \mathbf{j} \)](image-url)