4. Diffusion equations

As in the previous section, the central issue here is that of predicting the behavior of a function which measures the density of some type of particle as a function of time and position. At the beginning of the previous section, I derived a completely tautological equation for this function. Let me remind you: I use t to denote the time coordinate and x to denote the space coordinate; and then I use u to denote the function. Thus, u(t, x) measures the density of particles at time t and position x along some line. By keeping track of all possible fates of particles which start near x at time t, I argued that u should obey the equation

$$\frac{\partial}{\partial t}u(t, x) = -\frac{\partial}{\partial x}q(t, x) + k(t, x) . \tag{4.1}$$

Here,

- q(t, x) = (the number of particles per second crossing x from left to right at time t) - (the number of particles per second crossing x from right to left at time t) ,
- k(t, x) = (the number of particles per second per unit length which appear at x at time t) - (the number of particles per second per unit length which disappear at x at time t) .

(4.2)

With regard to (4.1), don't be misled by its stylish form, for (4.1) is only a fancy way of saying: "What comes in either stays in or goes out again". However, this equation can become useful when the functions q and k are specified.

For example, in the last section, I considered the case where the particle motion is due entirely to the movement of the ambient fluid. Under this last assumption, I argued that the appropriate choice for q(t, x) = c(t, x) u(t, x), where c(t, x) is the velocity of the fluid at time t and position x. (In the last section, I took c to be a constant, but that extra simplification is often a poor approximation to reality.) In the previous section, I also took k(t, x) to equal -r u(t, x), where r is a constant. The result of these choices yields the advection equation version of (4.1),

$$\frac{\partial}{\partial t}u(t, x) = - c \frac{\partial}{\partial x}u(t, x) - r u(t, x) , \tag{4.3}$$

whose general solution has the form

$$u(t, x) = e^{-rt} f(x - ct) \tag{4.4}$$

with f(·) any function you like of a single variable.

I can't stress enough that (4.3) is appropriate only when the particle motion is, to a good approximation, due only to the motion of the ambient fluid. This may not be the case. For example, the fluid may be at rest, and the particles might, individually have random motions. In the latter case, a different choice for the function q(t, x) is correct and the resulting version of (4.1) is called a <u>diffusion</u> <u>equation</u>.

a) The diffusion equation

The archetypal diffusion equation has the form

$$\frac{\partial}{\partial t}u = \mu \frac{\partial^2}{\partial x^2}u + k(t, x) \tag{4.5}$$

where k(t, x) is a function which can depend on u(t, x); and where μ is a constant which is determined by the average speed of the particles. Here, $\frac{\partial^2 u}{\partial x^2}$ signifies the second derivative of the function u along the x direction. (So, keep t fixed as if it were a constant and pretend that you are taking the derivatives of a function of x only.)

More precisely, the constant μ is determined by the square root of the average of the square of the velocity of the particles. The derivation of the number μ from first principles requires some fairly sophisticated probability theory. In practice, the constant μ can be measured in the laboratory using some fairly simple experiments. The constant μ is called the diffusion coefficient.

b) The derivation of the diffusion equation

Equation (4.5) is of the form of (4.1) with $q(t, x) = -\mu \frac{\partial}{\partial x} u(t, x)$. This general form for q can be justified in a heuristic sense as follows: When the motion of the particles is completely random, one expects that the number of particles which cross x per second at time t from left to right is proportional to the number of particles which are just to the left of x at time t. If the velocities of the particles are truly random, then roughly half of these particles will be moving to the right (and so not cross x), while half will be moving to the left, and so will cross x. Meanwhile, the number of particles per second which cross x from right to left at time t should be proportional to the number of particles which are just to the right of x at time t. Thus, we expect q(t, x) to be positive if there are more particles just to the left of x at time t then just to the right, and we expect q(t, x) to be negative if the converse is true. And, we expect q(t, x) to vanish if the number of particles just to the right is the same as the number which is just to the left. But, this is essentially saying that q(t, x) should be proportional to $-\frac{\partial}{\partial x} u(t, x)$, since $-\frac{\partial}{\partial x} u(t, x)$ is positive if there are more particles just to the left of x, and negative if there are more particles just to the right, and zero otherwise.

c) A fundamental solution

As with (4.3), the diffusion equation in (4.5) for any given form for k(t, x) has a whole raft of solutions. Of particular importance is the function

$$u(t, x) = \frac{a}{t^{1/2}} e^{-x^2/4\mu t} \tag{4.6}$$

which solves the k(t, x) = 0 version of (4.5):

$$\frac{\partial}{\partial t} u = \mu \frac{\partial^2}{\partial x^2} u \ . \tag{4.7}$$

In (4.6), a is any constant.

For any fixed t, the graph of u(t, x) in (4.6) is the standard "bell shaped curve", but as t increases, the curve gets flatter and flatter. (Its maximum height is at the origin, where $u(0, t) = a/t^{1/2}$. Thus, as t increases, the particle distribution does indeed diffuse out from a concentrated peak at small t to an almost uniformly small density at large t. See the sketches below:

(By the way, at any fixed time t, the integral of u(t, x) over the whole of the x axis is constant. This is predicted by (4.7) since the term k(t, x) which models the appearance and disappearance of particles is missing.)

d) The diffusion equation is predictive.

Somewhat more general then the k = 0 version of (4.5) is the case where the function k(t, x) = -r u(t, x). In this case, (4.5) reads

$$\frac{\partial}{\partial t} u = \mu \frac{\partial^2}{\partial x^2} u - r\, u \tag{4.8}$$

It is important to realize that the diffusion equation in (4.8), like the advection equation in (4.3), is <u>predictive</u> in the following sense:

Specify desired $t = 0$ *values for* u *as a function of* x*, and there is a unique solution* $u(t, x)$ *to (4.8) which has these given values at time* $t = 0$*. In particular, every solution to (4.8) is determined for all points* x *at all times* $t > 0$ *by its* $t = 0$ *values.*

This property of being predictive is what makes the diffusion equation and the advection equation so useful.

(The predictive nature of these equations can be proved by making rigorous the following argument: If you know $u(0, x)$, then the equation tells you what $\frac{\partial}{\partial t}u$ is at $t = 0$ and at any x. This tells you (approximately) $u(\Delta t, x)$ for small Δt and all x. (But, accuracy increases as Δt goes to zero.) Plug your new found knowledge of $u(\Delta t, x)$ into the left side of (1) or (2) to learn what $\frac{\partial}{\partial t}u$ is at $t = \Delta t$ and any x. This tells you (approximately) $u(2\Delta t, x)$ for small Δt and all x. Plug your new found knowledge of $u(2\Delta t, x)$ into the left side of (1) or (2) to learn what $\frac{\partial}{\partial t}u$ is at the next time step, $t = 2\Delta t$ and any x. . . . and so on and so on.)

For the advection equation, we saw already that the solution $u(t, x)$ is determined by its $t = 0$ values via the formula

$$u(t, x) = e^{-rt}\, u(0, x - ct) \quad . \tag{4.9}$$

Here, knowing $u(0, x)$ for all x explicitly allows you to compute $u(t, x)$ for any t and x.

For the diffusion equation in (4.8), the dependence of u(t, x) for $t \geq 0$ on the values of u at t = 0 has a more complicated form. In any event, here it is:

$$u(t, x) = \frac{1}{(4\pi\mu t)^{1/2}} e^{-rt} \int_{-\infty}^{\infty} u(0,s)\, e^{-(x-s)^2 / 4\mu t}\, ds . \tag{4.10}$$

In this last equation, you should think of the function $e^{-(x-s)^2 / 4\mu t}$ as a function of three variables, x, s and t. Then, (4.10) integrates over the s variable while keeping t and x fixed to obtain a function of x and t only.

e) Superposition

Both (4.3) and (4.8) obey the superposition principle. This principle goes as follows: Suppose that $u_1(t, x)$ and $u_2(t, x)$ are both solutions to either (4.3) or (4.8) and that a_1 and a_2 are numbers. Then

$$u(t, x) = a_1 u_1(t, x) + a_2 u_2(t, x) \tag{4.11}$$

is a solution to (4.3) or (4.8) as the case may be. This superposition principle is used over and over again in applications of these equations. (Equations for which the superposition principle holds are called linear equations. Generally, the superposition principle will fail if the equation involves powers of u greater than 1, or a function of u multiplying u or its derivatives or functions of derivatives of u multiplying derivatives of u. For example, the equation $\frac{\partial}{\partial t} u = \mu \frac{\partial^2}{\partial x^2} u + r u^2$ does not obey the superposition principle.)

Argue as follows to check the superposition principle for (4.3):

Step 1: Since a_1 and a_2 are constants, one computes

$$\frac{\partial}{\partial t}u = \frac{\partial}{\partial t}(a_1u_1 + a_2u_2) = a_1(\frac{\partial}{\partial t}u_1) + a_2(\frac{\partial}{\partial t}u_2) \quad . \tag{4.12}$$

This is because the derivative of a sum of function is the sum of the derivatives, and the derivative of a real number times a function is the real number times the derivative of the function.

<u>Step</u> <u>2</u>: Likewise, compute

$$\frac{\partial}{\partial x}u = \frac{\partial}{\partial x}(a_1u_1 + a_2u_2) = a_1(\frac{\partial}{\partial x}u_1) + a_2(\frac{\partial}{\partial x}u_2) \quad . \tag{4.13}$$

and multiply this last expression by -c to get

$$-c\frac{\partial}{\partial x}u = -c\frac{\partial}{\partial x}(a_1u_1 + a_2u_2) = a_1(-c\frac{\partial}{\partial x}u_1) + a_2(-c\frac{\partial}{\partial x}u_2). \tag{4.14}$$

<u>Step</u> <u>3</u>: Compute

$$r\,u = r\,(a_1u_1 + a_2u_2) = a_1(r\,u_1) + a_2\,(r\,u_2) \quad . \tag{4.15}$$

<u>Step</u> <u>4</u>: Add the right sides of (4.14) and (4.15), and likewise add the left sides of these equations. Since the right side of each is equal to the left side of each, you will find that

$$-c\,\frac{\partial}{\partial x}u + r\,u = a_1(-c\frac{\partial}{\partial x}u_1 + r\,u_1) + -a_2(-c\frac{\partial}{\partial x}u_2 + r\,u_2). \tag{4.16}$$

<u>Step</u> <u>5</u>: Finally, because u_1 and u_2 satisfy (4.3), the right hand side of (4.16) is equal to

$$a_1(\frac{\partial}{\partial t}u_1) + a_2(\frac{\partial}{\partial t}u_2) \tag{4.17}$$

which is the right side of (4.12). Thus, the right side of (4.17) is equal to $\frac{\partial}{\partial t}u$ as it has to be if u is to satisfy (4.13) as claimed.

Please convince yourself of the validity of the superposition principle for (4.8).

This superposition principle is <u>extremely</u> <u>important</u>. For example, the basic solution to (4.7) is

$$u_0(t, x) = \frac{1}{t^{1/2}} e^{-x^2/4\mu t} \tag{4.18}$$

or, more generally, if x_0 is any given point, then

$$u_{x_0}(t, x) = \frac{1}{t^{1/2}} e^{-(x-x_0)^2/4\mu t} \tag{4.19}$$

is a solution to (4.7). Using the superposition principle, I can immediately conclude that I can select any number of points $\{x_0, x_1, \ldots\}$ and a like number $\{a_0, a_1, \ldots\}$ of numbers (i.e. $x_0 = 12$, $x_1 = -2.4$, . . ., and $a_0 = 5$, $a_1 = -.3$, . . .) and then

$$a_0 \frac{1}{t^{1/2}} e^{-(x-x_0)^2/4\mu t} + a_1 \frac{1}{t^{1/2}} e^{-(x-x_1)^2/4\mu t} \ \ldots \tag{4.20}$$

is also a solution to (4.7).

d) Lessons

There are three important lessons to be had from this lecture:

- Under the assumption that the particles are moving randomly, (4.1) becomes (4.5), the diffusion equation
- Both (4.3) and (4.7)) are predictive in the following sense: Pick any function of the variable x, call it $u_0(x)$, and then both equations have a unique solution u(t, x) which equals your chosen function at t = 0. That is, $u(0, x) = u_0(x)$.
- Both equations obey the superposition principle. This is to say that if you have two solutions and you multiply each by a chosen number and add the resulting functions together, then the function of t and x so obtained also solves the equation.