28 Diffusion Equation: How irreversibility is captured

Our discussion on the diffusion equation in **1** relied very heavily on our physics intuition. We wish to see whether our intuition is correctly captured by the diffusion equation. The maximum principle tells us that the diffusion equation captures well irreversible nature of diffusion processes. This in turn implies that the diffusion problems are well-posed in Hadamard's sense. Diffusion equations allow infinite speed of propagation of signals and matter, but adding second order time derivative terms cure this unphysical nature.

Key words: maximum principle, well-posedness, preservation of order, infinite propagation speed, telegrapher's (Maxwell-Cattaneo) equation.

Summary:
(1) The solution to the diffusion equation evolves in time generally toward the more 'featureless' function. This is guaranteed by the maximum principle (**28.2**).
(2) When the solution of a problem is unique and depends on the auxiliary conditions continuously, the problems is said to be well-posed in the sense of Hadamard (**28.3**). Diffusion problems are well-posed (**28.4**).
(3) Diffusion equations allow infinite speed of propagation (**28.9**). Only the addition of higher order time derivatives can cure this (**28.10**).

28.1 Elementary summary. We have learned where diffusion equations appear (→**1.2**, **1.14**, **a1B.2**, **a1C.1**, **a1F.17**). Some Green's functions have been constructed (→**16B**), and we physically argued that if it exists, it is unique in the bounded domain in particular, under the following condition with a given initial field (→**1.18**):
(1) Dirichlet condition: At the boundary all the values of ψ are specified. For the heat conduction problem, this is the condition with the given wall temperature (i.e., thermostated).
(2) Neumann condition: At the boundary the normal derivative of ψ is given. For the heat conduction problem, this is the condition with the given heat flux through the wall.

We heavily relied on the zeroth law of thermodynamics: there is a unique equilibrium state if we wait long enough. Our argument is, however, in a certain sense circular, because we have shown that if the diffusion equation is physically reasonable, then we can rely on physics argument. To break this circle, we must demonstrate that indeed diffusion equation reflects thermodynamics correctly. This is equibvalent to demonstrating that our intuition and our mathematics could be in harmony (at least for the diffusion equation).

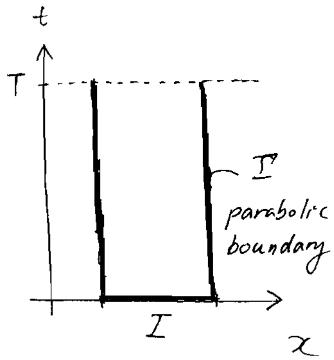
Exercise.
Solve

$$\frac{\partial u}{\partial t} = \Delta u + \boldsymbol{b} \cdot \nabla u + e^t \sin(x - b_x t), \tag{28.1}$$

with the initial condition $u(\boldsymbol{r}, 0) = |\boldsymbol{r}|$. Here $\boldsymbol{b}$ is a constant vector and b_x is its x-component.

28.2 Maximum principle. Let u be a solution[363] of the diffusion equation

$$u_t = u_{xx} \tag{28.2}$$



on $\Omega \equiv I \times [0, T]$, where I is an interval on the x-axis. Then, its maximum value is taken on the *parabolic boundary* $\Gamma = \partial I \times [0, T] \cup I \times \{0\}$. In particular, this means the maximum value of $|u|$ on I is a decreasing function of time.
[Demo] Let μ be the maximum value of u on the parabolic boundary Γ, and define

$$v = e^{-t}(u - \mu). \tag{28.3}$$

v satisfies

$$v_t + v = v_{xx} \tag{28.4}$$

in Ω°.[364] If we can prove that $v \le 0$ on Γ implies $v \le 0$ in $I^\circ \times (0, T]$, then we are almost done. Suppose v has a maximum value $v = v_0 > 0$ at $(x_0, t_0) \in \Omega^\circ$. At this point $v_{xx} \le 0$ and $v_t = 0$, so that (28.4) implies that $v_0 \le 0$, a contradiction. If there is a maximum at the boundary $t = T$, then $v_t \ge$ and $v_{xx} \le 0$, so $v < 0$. We are done.
(1) This principle also holds in d-space. An analogous demonstration works in any d-space, replacing I with a bounded region.
(2) As can be seen from the demonstration, if the solution may be assumed to be bounded everywhere, then the principle holds even if the problem is on an unbounded region.

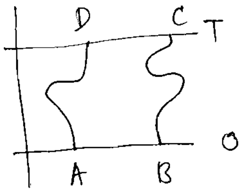
Discussion.
(1) What can you say about the evolution of the number of peaks of a solution to the diffusion equation (under, say, a time-independent Neumann condition)?

[363] There are actually several kinds of solutions. A solution in the ordinary sense of the calculus (requiring necessary differentiability, etc.), is called a *classical solution.*
[364] A° denotes the open kernel of the set A. That is, A° is the largest open set in A.

Gevrey's uniqueness theorem. Consider

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} + a(x,t)u = 0. \tag{28.5}$$

Here a is positive and continuous in the closed space time domain in the figure.[365] Let u be a solution to (28.5) that is continuous in the closed domain U considered above, satisfying (28.5) on the region $\hat{U} = U$ subtracted its parabolic boundary, and with continuous $\partial_t u$ and $\partial_x^2 u$ there. Then, u cannot have any positive maximum nor negative minimum in $\hat{U}$.□



[Demo]. Suppose we have a positive maximum inside DABC. Then, at the point

$$u > 0 \ \frac{\partial u}{\partial t} = 0, \ \frac{\partial^2 u}{\partial x^2} \le 0, \tag{28.6}$$

so that this contradicts $a > 0$. If there is a positive maximum on the open segment CD, then there,

$$u > 0 \ \frac{\partial u}{\partial t} \ge 0, \ \frac{\partial^2 u}{\partial x^2} \le 0, \tag{28.7}$$

This also contradicts $a > 0$. To show the statement about the minimum, consider $-u$ instead.

28.3 Well-posedness (in the sense of Hadamard).[366] Even if the unique solution exists, if the solution is extremely sensitive to the auxiliary conditions such as boundary and initial data, then the PDE may be useless for describing reproducible natural phenomena. A problem is said to be *well-posed (in the sense of Hadamard)*, if
(1) there is a solution which is unique,
and
(2) the solution depends continuously on the data (initial and other auxiliary conditions).

Otherwise, the problem is called *ill-posed.*[367] Physically reasonable problems are often well-posed as we will see later. For example, the Dirichlet problem for the Laplace equation is well-posed (→**29.9**).[368]

The existence of a solution implies that the problem is not *overdetermined.* The uniqueness of the solution implies that the problem is

[365] A and B can be coincident. Furthermore, the side curves can wiggle wildly so long as they do not cross the upper and lower lines.

[366] Jacque Salomon Hadamard, 1865-1963. Read J. Hadamard, *The Psychology of Invention in the Mathematical Field* (Dover, 1945) on creativity.

[367] The condition (2) must be stated more precisely with the aid of some norm (→**3.3** footnote) to make the concept 'continuous' meaningful.

[368] One might suggests that chaos is an example of the lack of well-posedness, but most examples of chaos are well-posed, because the continuous dependence of the solution on the initial condition is trivially satisfied for any finite time.

not *underdetermined.*

28.4 Cauchy problem of diffusion equation with Dirichlet condition is well-posed. That is, the solution is unique and depends continuously on the initial and boundary data. [This theorem is proved for a bounded region here. Also we will not discuss the existence of a solution.]

[Demo] Let u_1 and u_2 be two solutions of the same problem. Then, due to the linearity of the problem, the difference $u = u_1 - u_2$ obeys the same diffusion equation with a homogeneous Dirichlet boundary condition (i.e., $u = 0$ at the boundary of the domain) and $u = 0$ initially as we have discussed (→**1.18**). From the maximum principle u cannot be larger than 0, and $-u$ cannot be larger than 0. Hence, $u_1 = u_2$. That is, if there is a solution, it is unique. Now, we compare two different problems 1 and 2 with the auxiliary conditions which are different slightly. Let the solutions of 1 and 2 be u_1 and u_2, respectively. Then, the maximum principle tells us that the maximum value of $|u_1 - u_2|$ in the region cannot be larger than the differences in the initial and boundary data. Hence, the solution depends on the auxiliary conditions continuously.[369] That is, the problem is well posed in Hadamard's sense.

Exercise.
Show that $\int u \ln u dx$ is non-increasing, if u obeys a diffusion equation. Assume the initial $u \geq 0$, and consider the problem in $\boldsymbol{R}^2$.

28.5 Anti-diffusion: violation of second law. Thermodynamically destabilizing the world can produce ill-posed problems. A typical example is the 'anti'-diffusion equation.

$$\frac{\partial u}{\partial y} + \frac{\partial^2 u}{\partial x^2} = 0 \tag{28.8}$$

Notice that the amplitude of the mode e^{ikx} is amplified as $e^{+k^2 y}$, so unless the initial data decay faster than this factor in k-space, a kind of Hadamard instability occurs for any finite 'time' $y > 0$.[370]

Discussion.

$$\frac{\partial u}{\partial t} + t\frac{\partial^2 u}{\partial x^2} = f(x,t) \tag{28.9}$$

cannot make a well-posed problem. The reason should be obvious.[371]

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[369]That is, when the sup norm of the change in the auxiliary condition is made small indefinitely, so does the sup norm of the corresponding change of the solution.

[370]As we have seen, the ill-posedness of a problem is closely related to instability in the ultraviolet limit ($k \to \infty$).

[371]Y. Kannai, Israel J. Math. **9**, 306 (1971).

28.6 Preservation of order, positivity. Let u_1 and u_2 be two solutions of the diffusion equation on the domain Ω as in **28.2**. If $u_1 \leq u_2$ on the parabolic boundary (→**28.2**), then $u_1 \leq u_2$ in $\Omega°$. Hence, for example, if $u_1 \leq u_2$ at $t = 0$, then this relation holds forever. In particular, if the initial condition is positive and the boundary value is non-negative, then the solution is positive forever. This should be obvious from the maximum principle.

28.7 Spatially inhomogeneous and/or anisotropic diffusion. Physically, the consequences of irreversibility should not be affected by the existence of spatial inhomogeneity and/or anisotropy (with time-dependence). We encounter the following equation in such a case (with the summation convention):

$$\frac{\partial u}{\partial t} = a_{ij}(x,t)\frac{\partial^2 u}{\partial x_i \partial x_j} + b_i(x,t)\frac{\partial u}{\partial x_i} + c(x,t)u \tag{28.10}$$

or its divergence form (with different coefficient functions):

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x_i}a_{ij}(x,t)\frac{\partial u}{\partial x_j} + b_i(x,t)\frac{\partial u}{\partial x_i} + c(x,t)u. \tag{28.11}$$

The second law requires the positive definiteness of the matrix $Matr(a_{ij})$. Under this condition it is known that so long as $c \leq 0$ the maximum principle (→**28.2**) holds. Thus everything we can conclude intuitively about diffusion based on thermodynamics should also be captured in the spatially inhomogeneous diffusion equation. It is physically very sensible that the existence of the advection (→**2B.6**) term b is irrelevant to the maximum principle.

28.8 Unbounded space. So far we have heavily relied on the boundedness of the domain of the problem. Note that the diffusion equation can have a rapidly growing solution even if the initial data is zero $u(x, 0) = 0$ as Tikhonov demonstrated.[372] See also the warning in **1.18**(5). In any case, this episode tells us a danger of mathematical modeling: since diffusion equations are derived as a balance condition of conserved quantities (→**a1B.2**), it is physically unthinkable that initially everywhere 0 solution can grow (However, if the growth rate of the solution as a function of x is not too rapid, then the initial value problem can be solved uniquely. In particular, a bounded solution is unique.)

28.9 Infinite propagation speed. For a very short time, the solution of the diffusion equation is almost independent of the (bounded)

[372] F. John, p211-3.

boundary condition away from the boundary, and is given by (3.6). In particular, if the thermal energy is concentrated at the origin at $t = 0$ (i.e., $T(\boldsymbol{x}, 0) = \delta(\boldsymbol{x})$ →**14.5**):

$$T(\boldsymbol{x}, t) = \frac{1}{\sqrt{4\pi t}^d} e^{-x^2/4t} \tag{28.12}$$

is an accurate solution of $\partial_t T = \Delta T$ for short time in d-space (→**16B.1**). For any positive t, however small it may be, $T(x, t) > 0$ for any x. Thus we must conclude that heat can travel at infinite speed. This is true for the diffusion equation for chemical species as well. This is physically unrealistic. However, for most applications of diffusion equations, this is good enough because the tail part of T is much smaller than exponentially small quantities, and because significant error could occur only for extremely short times (when a collective description like diffusion is not applicable).

28.10 Short-time modification of diffusion equation: the Maxwell-Cattaneo equation.[373] We must modify the diffusion equation, if we wish to describe the short time behavior of the system more realistically. This is only possible by adding higher order time derivatives.[374] Hence, the following modification has been proposed:

$$c\frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = D_T \Delta T, \tag{28.13}$$

where c is a positive constant. This is called, in the context of heat conduction, the *Maxwell-Cattaneo equation.* We have already come across this type of equation in conjunction to the propagation of electromagnetic wave in matter (e.g., the telegrapher's equation →**a1F.17**). Therefore, obviously, infinite speed of propagation is eliminated.[375]

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[373] cf. Compt. Rend. **247**, 431 (1958).

[374] In Newton's equation of motion, the inertial effect is described by the second order time derivative, and the dissipative effect by the first order time derivative as in $\ddot{x} = -\eta\dot{x} + f$, where η is the friction constant, and f an external driving force. If we pay our attention only to the very short time behavior of the system, we do not see the dissipation term. The effect of dissipation sets in only later. Such an observation is also important in hydrodynamics. The Euler equation (→**a1E.7**) accurately describes the initial motion of a body in a viscous fluid under impulsive force.

[375] The equation now becomes a hyperbolic equation (→**1.20**). One of the important properties of hyperbolic equations is the finiteness of the propagation speed (→**30.16**).