Entropy and Partial Differential Equations

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Inspiring Quotations

A good many times I have been present at gatherings of people who, by the standards of traditional culture, are thought highly educated and who have with considerable gusto been expressing their incredulity at the illiteracy of scientists. Once or twice I have been provoked and have asked the company how many of them could describe the Second Law of Thermodynamics. The response was cold: it was also negative. Yet I was asking something which is about the scientific equivalent of: Have you read a work of Shakespeare's?

–C. P. Snow, *The Two Cultures and the Scientific Revolution*

. . . C. P. Snow relates that he occasionally became so provoked at literary colleagues who scorned the restricted reading habits of scientists that he would challenge them to explain the second law of thermodynamics. The response was invariably a cold negative silence. The test was too hard. Even a scientist would be hard-pressed to explain Carnot engines and refrigerators, reversibility and irreversibility, energy dissipation and entropy increase. . . all in the span of a cocktail party conversation.

–E. E. Daub, "Maxwell's demon"

He began then, bewilderingly, to talk about something called entropy . . . She did gather that there were two distinct kinds of this entropy. One having to do with heat engines, the other with communication. . . "Entropy is a figure of speech then". . . "a metaphor".

–T. Pynchon, *The Crying of Lot 49*

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INTRODUCTION

A. Overview

This course surveys various uses of "entropy" concepts in the study of PDE, both linear and nonlinear. We will begin in Chapters I–III with a recounting of entropy in physics, with particular emphasis on axiomatic approaches to entropy as

(i) characterizing *equilibrium* states (Chapter I),

(ii) characterizing *irreversibility* for processes (Chapter II),

and

(iii) characterizing *continuum* thermodynamics (Chapter III).

Later we will discuss probabilistic theories for entropy as

(iv) characterizing *uncertainty* (Chapter VII).

I will, especially in Chapters II and III, follow the mathematical derivation of entropy provided by modern rational thermodynamics, thereby avoiding many customary physical arguments. The main references here will be Callen [C], Owen [O], and Coleman–Noll [C-N]. In Chapter IV I follow Day [D] by demonstrating for certain linear second-order elliptic and parabolic PDE that various estimates are analogues of entropy concepts (e.g. the Clausius inequality). I as well draw connections with Harnack inequalities. In Chapter V (conservation laws) and Chapter VI (Hamilton–Jacobi equations) I review the proper notions of weak solutions, illustrating that the *in*equalities inherent in the definitions can be interpreted as irreversibility conditions. Chapter VII introduces the probabilistic interpretation of entropy and Chapter VIII concerns the related theory of large deviations. Following Varadhan [V] and Rezakhanlou [R], I will explain some connections with entropy, and demonstrate various PDE applications.

B. Themes

In spite of the longish time spent in Chapters I–III, VII reviewing physics, this is a mathematics course on partial differential equations. My main concern is PDE and how various notions involving entropy have influenced our understanding of PDE. As we will cover a lot of material from many sources, let me explicitly write out here some unifying themes:

(i) the use of entropy in *deriving* various physical PDE,

(ii) the use of entropy to characterize *irreversibility* in PDE evolving in time,

and

(iii) the use of entropy in providing *variational principles*.

Another ongoing issue will be

(iv) understanding the relationships between entropy and *convexity*.

I am as usual very grateful to F. Yeager for her quick and accurate typing of these notes.

CHAPTER 1: Entropy and equilibrium

A. Thermal systems in equilibrium

We start, following Callen [C] and Wightman [W], by introducing a simple mathematical structure, which we will later interpret as modeling *equilibria of thermal systems*:

Notation. We denote by $(X_0, X_1, \ldots, X_m)$ a typical point of $\mathbb{R}^{m+1}$, and hereafter write

$$E = X_0.$$

□

A model for a thermal system in equilibrium

Let us suppose we are given:

(a) an open, convex subset Σ of $\mathbb{R}^{m+1}$,

and

(b) a C^1-function

$$S : \Sigma \to \mathbb{R} \tag{1}$$

such that

$$\begin{cases} \text{(i)} & S \text{ is concave} \\ \text{(ii)} & \frac{\partial S}{\partial E} > 0 \\ \text{(iii)} & S \text{ is positively homogeneous of degree 1.} \end{cases} \tag{2}$$

We call Σ the *state space* and S the *entropy* of our system:

$$S = S(E, X_1, \ldots, X_m) \tag{3}$$

Here and afterwards we assume without further comment that S and other functions derived from S are evaluated only in open, convex regions where the various functions make sense. In particular, when we note that (2)(iii) means

$$S(\lambda E, \lambda X_1, \ldots, \lambda X_m) = \lambda S(E, X_1, \ldots, X_m) \qquad (\lambda > 0), \tag{4}$$

we automatically consider in (4) only those states for which both sides of (4) are defined.

Owing to (2)(ii), we can solve (3) for E as a C^1 function of $(S, X_1, \ldots, X_m)$:

$$E = E(S, X_1, \ldots, X_m). \tag{5}$$

We call the function E the *internal energy*.

Definitions.

$$\begin{aligned} T &= \tfrac{\partial E}{\partial S} = \textit{ temperature} \\ P_k &= -\tfrac{\partial E}{\partial X_k} = \textit{ } k^{th} \textit{ generalized force} \text{ (or } \textit{pressure}). \end{aligned} \tag{6}$$

Lemma 1 (i) *The function E is positively homogeneous of degree 1:*

$$E(\lambda S, \lambda X_1, \dots, \lambda X_m) = \lambda E(S, X_1, \dots, X_m) \quad (\lambda > 0). \tag{7}$$

(ii) *The functions T, P_k $(k = 1, \dots)$ are positively homogeneous of degree 0:*

$$\begin{cases} T(\lambda S, \lambda X_1, \dots, \lambda X_m) = T(S, X_1, \dots, X_m) \\ P_k(\lambda S, \lambda X_1, \dots, \lambda X_m) = P_k(S, X_1, \dots, X_m) \quad (\lambda > 0). \end{cases} \tag{8}$$

We will later interpret (2), (7) physically as saying the S, E are *extensive parameters* and we say also that $X_1, \dots, X_n$ are extensive. By contrast (8) says T, P_k are *intensive parameters.*

Proof. 1. $W = E(S(W, X_1, \dots, X_m), X_1, \dots, X_m)$ for all $W, X_1, \dots, X_m$. Thus

$$\begin{aligned} \lambda W &= E(S(\lambda W, \lambda X_1, \dots, \lambda X_m), \lambda X_1, \dots, \lambda X_m) \\ &= E(\lambda S(W, X_1, \dots, X_m), \lambda X_1, \dots, \lambda X_m) \text{ by (4).} \end{aligned}$$

Write $S = S(W, X_1, \dots, X_m)$, $W = E(S, X_1, \dots, X_m)$ to derive (7).

2. Since S is C^1, so is E. Differentiate (7) with respect to S, to deduce

$$\lambda \frac{\partial E}{\partial S}(\lambda S, \lambda X_1, \dots, \lambda X_m) = \lambda \frac{\partial E}{\partial S}(S, X_1, \dots, X_m).$$

The first equality in (8) follows from the definition $T = \frac{\partial E}{\partial S}$. The other equalities in (8) are similar. □

Lemma 2 *We have*

$$\frac{\partial S}{\partial E} = \frac{1}{T}, \ \frac{\partial S}{\partial X_k} = \frac{P_k}{T} \quad (k = 1, \dots, m). \tag{9}$$

Proof. $T = \frac{\partial E}{\partial S} = \left(\frac{\partial S}{\partial E}\right)^{-1}$. Also

$$W = E(S(W, X_1, \dots, X_m), X_1, \dots, X_m)$$

for all $W, X_1, \dots, X_m$. Differentiate with respect to X_k:

$$0 = \underbrace{\frac{\partial E}{\partial S}}_{=T} \frac{\partial S}{\partial X_k} + \underbrace{\frac{\partial E}{\partial X_k}}_{=-P_k}.$$

□

We record the definitions (6) by writing

$$dE = TdS - \sum_{k=1}^{m} P_k dX_k \qquad \textit{Gibbs' formula.} \tag{10}$$

Note carefully: at this point (10) means merely $T = \frac{\partial E}{\partial S}$, $P_k = -\frac{\partial E}{\partial X_k}$ $(k = 1, \ldots, m)$. We will later in Chapter II interpret TdS as "infinitesimal heating" and $\sum_{k=1}^{m} P_k dX_k$ as "infinitesimal working" for a process. In this chapter however there is no notion whatsoever of anything changing in time: everything is in equilibrium.

Terminology. The formula

$$S = S(E, X_1, \ldots, X_m)$$

is called the *fundamental equation* of our system, and by definition contains all the thermodynamic information. An identity involving other derived quantities (i.e. T, P_k $(k = 1, \ldots, m)$) is an *equation of state*, which typically does not contain all the thermodynamic information. □

B. Examples

In applications $X_1, \ldots, X_m$ may measure many different physical quantities.

1. Simple fluid. An important case is a *homogeneous simple fluid*, for which

$$\begin{aligned} E &= \textit{internal energy} \\ V &= \textit{volume} \\ N &= \textit{mole number} \\ S &= S(E, V, N) \\ T &= \tfrac{\partial E}{\partial S} = \textit{temperature} \\ P &= -\tfrac{\partial E}{\partial V} = \textit{pressure} \\ \mu &= -\tfrac{\partial E}{\partial N} = \textit{chemical potential.} \end{aligned} \tag{1}$$

So here we take $X_1 = V$, $X_2 = N$, where N measures the amount of the substance comprising the fluid. Gibbs' formula reads:

$$dE = TdS - PdV - \mu dN. \tag{2}$$

Remark. We will most often consider the situation that N is identically constant, say $N = 1$. Then we write

$$S(E, V) = S(E, V, 1) = \text{ entropy/mole}, \tag{3}$$

and so

$$
\begin{aligned}
E &= \text{internal energy} \\
V &= \text{volume} \\
S &= S(E,V) = \text{ entropy} \\
T &= \tfrac{\partial E}{\partial S} = \text{ temperature} \\
P &= -\tfrac{\partial E}{\partial V} = \text{ pressure}
\end{aligned} \tag{4}
$$

with

$$dE = TdS - PdV. \tag{5}$$

Note that $S(E,V)$ will not satisfy the homogeneity condition (2)(iii) however. □

Remark. If we have instead a *multicomponent simple fluid*, which is a uniform mixture of r different substances with mole numbers $N_1, \ldots, N_r$, we write

$$
\begin{aligned}
S &= S(E,V,N_1,\ldots,N_r) \\
\mu_j &= -\tfrac{\partial E}{\partial N_j} = \textit{ chemical potential of } j^{th} \textit{ component.}
\end{aligned}
$$

□

2. Other examples. Although we will for simplicity of exposition mostly discuss simple fluid systems, it is important to understand that many interpretations are possible. (See, e.g., Zemansky [Z].)

Extensive parameter X	Intensive parameter $P = -\frac{\partial E}{\partial X}$
length	tension
area	surface tension
volume	pressure
electric charge	electric force
magnetization	magnetic intensity

Remark. Again to foreshadow, we are able in all these situations to interpret:

$$PdX = \text{“infinitesimal work” performed by the system during some process}$$

↗ “generalized force” ↖ “infinitesimal displacement”

□

C. Physical interpretations of the model

In this section we provide some nonrigorous physical arguments supporting our model in §A of a thermal system in equilibrium. We wish therefore to explain why we suppose

$$\begin{cases} \text{(i)} & S \text{ is concave} \\ \text{(ii)} & \frac{\partial S}{\partial E} > 0 \\ \text{(iii)} & S \text{ is positively homogeneous of degree 1.} \end{cases}$$

(See Appendix B for statements of "physical postulates".)

1. Equilibrium

First of all we are positing that the "thermal system in equilibrium" can be completely described by specifying the $(m+1)$ macroscopic parameters $X_0, X_1, \ldots, X_m$, of which $E = X_0$, the internal energy, plays a special role. Thus we imagine, for instance, a body of fluid, for which there is no temporal or spatial dependence for $E, X_1, \ldots, X_m$.

2. Positivity of temperature

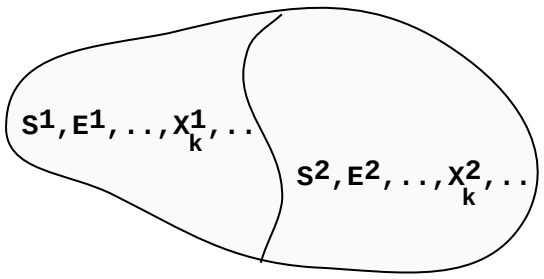
Since $\frac{\partial S}{\partial E} = \frac{1}{T}$, hypothesis (ii) is simply that *the temperature is always positive.*

3. Extensive and intensive parameters

The homogeneity condition (iii) is motivated as follows. Consider for instance a fluid body in equilibrium for which the energy is E, the entropy is S, and the other extensive parameters are X_k $(k = 1, \ldots, m)$.

Next consider a subregion # 1, which comprises a λ^{th} fraction of the entire region $(0 < \lambda < 1)$. Let $S^1, E^1, \ldots, X_k^1$ be the extensive parameters for the subregion. Then

$$(1) \qquad \begin{cases} S^1 &= \lambda S \\ E^1 &= \lambda E \\ X_k^1 &= \lambda X_k \qquad (k = 1, \ldots, m) \end{cases}$$



Consider as well the complementary subregion # 2, for which

$$\left\{\begin{array}{rcll} S^2 &=& (1-\lambda)S & \\ E^2 &=& (1-\lambda)E & \\ X_k^2 &=& (1-\lambda)X_k & (k=1,\dots,m). \end{array}\right.$$

Thus

$$\left\{\begin{array}{rcl} S &=& S^1+S^2 \\ E &=& E^1+E^2 \\ X_k &=& X_k^1+X_k^2 \quad (k=1,\dots,m). \end{array}\right. \tag{2}$$

The homogeneity assumption (iii) is just (1). As a consequence, we see from (2) that $S, E, \dots, X_m$ are *additive over subregions* of our thermal system in equilibrium.

On the other hand, if $T^1, P_k^1, \dots$ are the temperatures and generalized forces for subregion # 1, and $T^2, \dots, P_k^2, \dots$ are the same for subregion # 2, we have

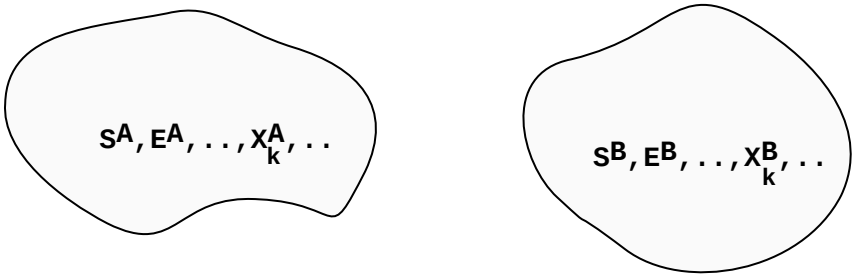
$$\left\{\begin{array}{rcccl} T &=& T^1 &=& T^2 \\ P_k &=& P_k^1 &=& P_k^2 \quad (k=1,\dots,m), \end{array}\right.$$

owing to Lemma 1 in §A. Hence $T, \dots, P_k$ are *intensive parameters*, which take the same value on each subregion of our thermal system in equilibrium.

4. Concavity of S

Note very carefully that we are hypothesizing the additivity condition (2) only for *subregions* of a given thermal system in equilibrium.

We next motivate the concavity hypothesis (i) by looking at the quite different physical situation that we have two *isolated* fluid bodies A, B of the same substance:



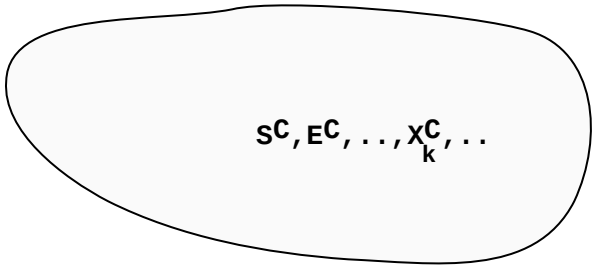
Here

$$\left\{\begin{array}{l} S^A = S(E^A,\dots,X_k^A,\dots) = \text{ entropy of } A \\ S^B = S(E^B,\dots,X_k^B,\dots) = \text{ entropy of } B, \end{array}\right.$$

for the same function $S(\cdot, \cdots)$. The total entropy is

$$S^A + S^B.$$

We now ask what happens when we "combine" A and B into a new system C, in such a way that no work is done and no heat is transferred to or from the surrounding environment:



(In Chapter II we will more carefully define "heat" and "work".) After C reaches equilibrium, we can meaningfully discuss $S^C, E^C, \ldots, X_k^C, \ldots$. Since no work has been done, we have

$$X_k^C = X_k^A + X_k^B \qquad (k = 1, \ldots, m)$$

and since, in addition, there has been no heat loss or gain,

$$E^C = E^A + E^B.$$

This is a form of the First Law of thermodynamics.

We however do *not* write a similar equality for the entropy S. Rather we invoke the Second Law of thermodynamics, which implies that entropy cannot decrease during any irreversible process. Thus

$$S^C \geq S^A + S^B. \tag{3}$$

But then

$$\begin{aligned} S^C &= S(E^C, \ldots, X_k^C, \ldots) \\ &= S(E^A + E^B, \ldots, X_k^A + X_k^B, \ldots) \\ &\geq S^A + S^B \\ &= S(E^A, \ldots, X_k^A, \ldots) + S(E^B, \ldots, X_k^B, \ldots). \end{aligned} \tag{4}$$

This inequality implies S is a concave function of $(E, X_1, \ldots, X_m)$. Indeed, if $0 < \lambda < 1$, we have:

$$\begin{aligned} &S(\lambda E^A + (1-\lambda)E^B, \ldots, \lambda X_k^A + (1-\lambda)X_k^B, \ldots) \\ &\geq S(\lambda E^A, \ldots, \lambda X_k^A, \ldots) + S((1-\lambda)E^B, \ldots, (1-\lambda)X_k^B, \ldots) \text{ by (4)} \\ &= \lambda S(E^A, \ldots, X_k^A, \ldots) + (1-\lambda)S(E^B, \ldots, X_k^B, \ldots) \text{ by (iii)}. \end{aligned}$$

Thus S is concave.

5. Convexity of E

Next we show that

$$E \text{ is a convex functionof } (S, X_1, \dots, X_m). \tag{5}$$

To verify (5), take any $S^A, S^B, X_1^A, \dots, X_m^A, X_1^B, \dots, X_m^B$, and $0 < \lambda < 1$. Define

$$\begin{cases} E^A := E(S^A, X_1^A, \dots, X_m^A) \\ E^B := E(S^B, X_1^B, \dots, X_m^B); \end{cases}$$

so that

$$\begin{cases} S^A = S(E^A, X_1^A, \dots, X_m^A) \\ S^B = S(E^B, X_1^B, \dots, X_m^B). \end{cases}$$

Since S is concave,

$$\begin{aligned} & S(\lambda E^A + (1-\lambda)E^B, \dots, \lambda X_k^A + (1-\lambda)X_k^B, \dots) \\ & \geq \lambda S(E^A, \dots, X_k^A, \dots) \\ & +(1-\lambda)S(E^B, \dots, X_k^B, \dots). \end{aligned} \tag{6}$$

Now

$$W = E(S(W, \dots, X_k, \dots), \dots, X_k, \dots)$$

for all $W, X_1, \dots, X_m$. Hence

$$\begin{aligned} \lambda E^A + (1-\lambda)E^B &= E(S(\lambda E^A + (1-\lambda)E^B, \dots, \lambda X_k^A \\ &\quad +(1-\lambda)X_k^B, \dots), \dots, \lambda X_k^A + (1-\lambda)X_k^B, \dots) \\ &\geq E(\lambda S(E^A, \dots, X_A^k, \dots) \\ &\quad +(1-\lambda)S(E^B, \dots, X_k^B, \dots), \dots, \lambda X_k^A + (1-\lambda)X_k^B, \dots) \end{aligned}$$

owing to (6), since $\frac{\partial E}{\partial S} = T > 0$. Rewriting, we deduce

$$\begin{aligned} & \lambda E(S^A, \dots, X_k^A, \dots) + (1-\lambda)E(S^B, \dots, X_k^B, \dots) \\ & \geq E(\lambda S^A + (1-\lambda)S^B, \dots, \lambda X_k^A + (1-\lambda)X_k^B, \dots), \end{aligned}$$

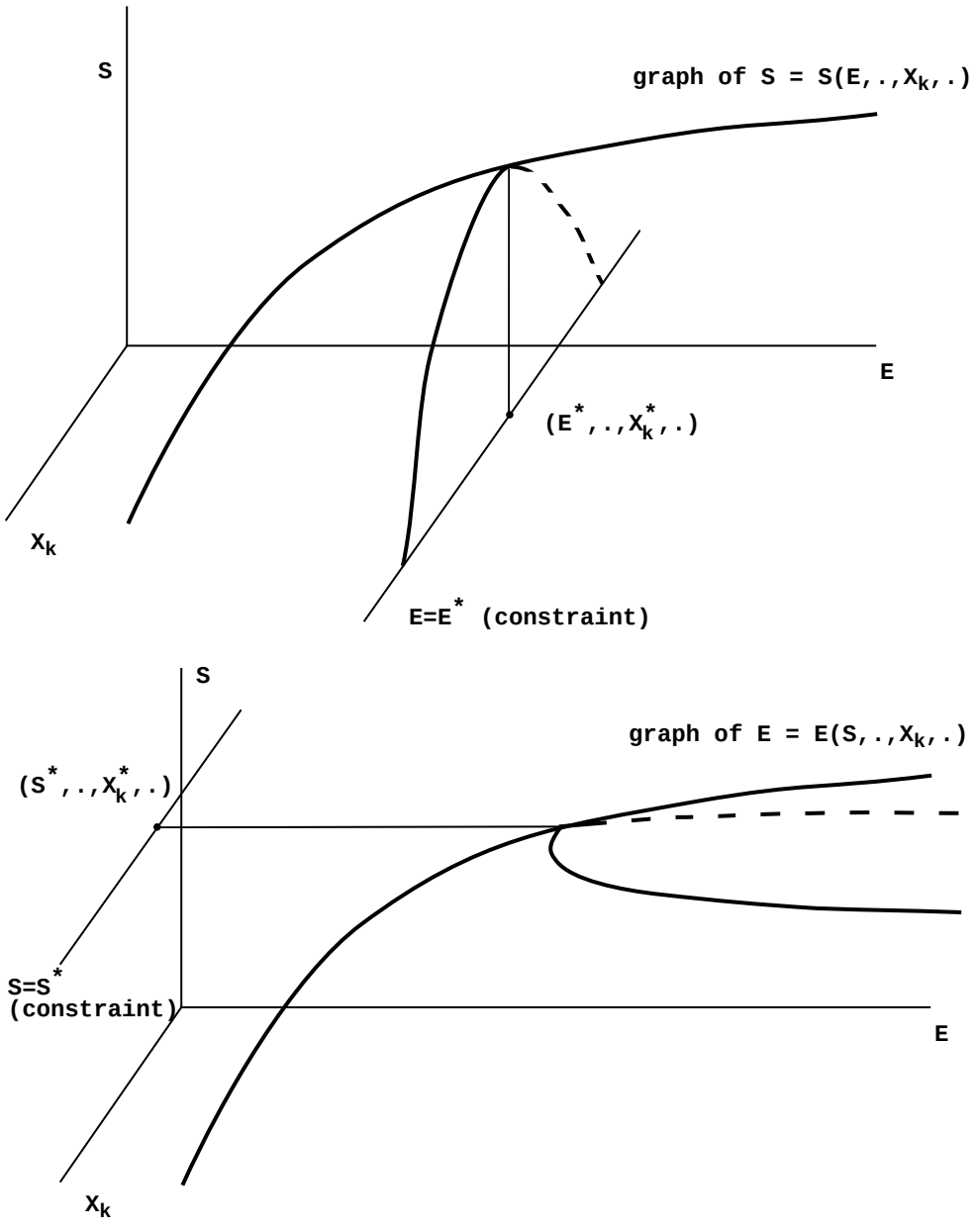
and so E is convex. □

6. Entropy maximization and energy minimization

Lastly we mention some physical variational principles (taken from Callen [C, p. 131–137]) for *isolated thermal systems*.

Entropy Maximization Principle. The equilibrium value of any unconstrained internal parameter is such as to *maximize the entropy* for the given value of the total internal energy.

Energy Minimization Principle. The equilibrium value of any unconstrained internal parameter is such as to *minimize the energy* for the given value of the total entropy.



The first picture illustrates the entropy maximization principle: Given the energy constraint $E = E^*$, the values of the unconstrained parameters $(X_1, \ldots, X_m)$ are such as to maximize

$$(X_1, \ldots, X_m) \mapsto S(E^*, X_1, \ldots, X_m).$$

The second picture is the "dual" energy minimization principle. Given the entropy constraint $S = S^*$, the values of the unconstrained parameters $(X_1, \ldots, X_m)$ are such as to minimize

$$(X_1, \ldots, X_m) \mapsto E(S^*, X_1, \ldots, X_m).$$

D. Thermodynamic potentials

Since E is convex and S is concave, we can employ ideas from convex analysis to rewrite various formulas in terms of the intensive variables $T = \frac{\partial E}{\partial S}$, $P_k = -\frac{\partial E}{\partial X_k}$ $(k = 1, \ldots, m)$. The primary tool will be the Legendre transform. (See e.g. Sewell [SE], [E1, §III.C], etc.)

1. Review of Legendre transform

Assume that $H : \mathbb{R}^n \to (-\infty, +\infty]$ is a convex, lower semicontinuous function, which is proper (i.e. not identically equal to infinity).

Definition. The *Legendre transform* of L is

$$L(q) = \sup_{p \in \mathbb{R}^n} (p \cdot q - H(p)) \qquad (q \in \mathbb{R}^n). \tag{1}$$

We usually write $L = H^*$. It is not very hard to prove that L is likewise convex, lower semicontinuous and proper. Furthermore the Legendre transform of $L = H^*$ is H:

$$L = H^*, \ H = L^*. \tag{2}$$

We say H and L are *dual* convex functions.

Now suppose for the moment that H is C^2 and is strictly convex (i.e. $D^2 H > 0$). Then, given q, there exists a unique point p which maximizes the right hand side of (1), namely the unique point $p = p(q)$ for which

$$q = DH(p). \tag{3}$$

Then

$$L(q) = p \cdot q - H(p), \ p = p(q) \text{ solving (3)}. \tag{4}$$

Furthermore

$$\begin{aligned} DL(q) &= p + (q - DH(p))D_q p \\ &= p \text{ by (3)}, \end{aligned}$$

and so

$$p = DL(q). \tag{5}$$

Remark. In mechanics, H often denotes the *Hamiltonian* and L the *Lagrangian*. □

2. Definitions

The energy E and entropy S are not directly physically measurable, whereas certain of the intensive variables (e.g. T, P) are. It is consequently convenient to employ the Legendre transform to convert to functions of various intensive variables. Let us consider an energy function

$$E = E(S, V, X_2, \ldots, X_m),$$

where we explicitly take $X_1 = V =$ volume and regard the remaining parameters $X_2, \ldots, X_m$ as being fixed. For simplicity of notation, we do not display $(X_2, \ldots, X_m)$, and just write

$$E = E(S, V). \tag{6}$$

There are 3 possible Legendre transforms, according as to whether we transform in the variable S only, in V only, or in (S, V) together. Because of sign conventions (i.e. $T = \frac{\partial E}{\partial S}$ $P = -\frac{\partial E}{\partial V}$) and because it is customary in thermodynamics to take the *negative* of the mathematical Legendre transform, the relevent formulas are actually these:

Definitions. (i) The *Helmholtz free energy* F is

$$F(T, V) = \inf_S (E(S, V) - TS).^1 \tag{7}$$

(ii) The *enthalpy* H is

$$H(S, P) = \inf_V (E(S, V) + PV). \tag{8}$$

(iii) The *Gibbs potential* (a.k.a. *free enthalpy*) is

$$G(T, P) = \inf_{S,V} (E(S, V) + PV - ST). \tag{9}$$

The functions E, F, G, H are called *thermodynamic potentials*.

[1]The symbol A is also used to denote the Helmholtz free energy.

Remark. The "inf" in (7) is taken over those S such that (S, V) lies in the domain of E. A similar remark applies to (8), (9). □

To go further we henceforth assume:

$$E \text{ is } C^2, \text{ strictly convex} \tag{10}$$

and furthermore that for the range of values we consider

$$\begin{cases} \text{the "inf" in each of (7), (8), (9) is attained at} \\ \text{a unique point in the domain of } E. \end{cases} \tag{11}$$

We can then recast the definitions (7)–(9):

Thermodynamic potentials, rewritten:

$$F = E - TS, \text{ where } T = \frac{\partial E}{\partial S} \tag{12}$$

$$H = E + PV, \text{ where } P = -\frac{\partial E}{\partial V} \tag{13}$$

$$G = E - TS + PV, \text{ where } T = \frac{\partial E}{\partial S},\ P = -\frac{\partial E}{\partial V}. \tag{14}$$

More precisely, (12) says $F(T, V) = E(S, V) - TS$, where $S = S(T, V)$ solves $T = \frac{\partial E}{\partial S}(S, V)$. We are assuming we can uniquely, smoothly solve for $S = S(T, V)$.

Commentary. If E is not strictly convex, we cannot in general rewrite (7)–(9) as (12)–(14). In this case, for example when the graph of E contains a line or plane, the geometry has the physical interpretation of *phase transitions*: see Wightman [W]. □

Lemma 3

(i) *E is locally strictly* convex *in* (S, V).
(ii) *F is locally strictly* concave *in T, locally strictly* convex *in V.*
(iii) *H is locally strictly* concave *in P, locally strictly* convex *in S.*
(iv) *G is locally strictly* concave *in* (T, P).

Remark. From (9) we see that G is the inf of affine mappings of (T, P) and thus is concave. However to establish the strict concavity, etc., we will invoke (10), (11) and use the formulations (12)–(14). Note also that we say "locally strictly" convex, concave in (ii)–(iv), since what we really establish is the sign of various second derivatives. □

Proof. 1. First of all, (i) is just our assumption (10).

2. To prove (ii), we recall (12) and write

$$F(T,V) = E(S(T,V),V) - TS(T,V), \tag{15}$$

where

$$T = \frac{\partial E}{\partial S}(S(T,V),V). \tag{16}$$

Then (15) implies

$$\begin{cases} \frac{\partial F}{\partial T} = \frac{\partial E}{\partial S}\frac{\partial S}{\partial T} - S - T\frac{\partial S}{\partial T} = -S \\ \frac{\partial F}{\partial V} = \frac{\partial E}{\partial S}\frac{\partial S}{\partial V} + \frac{\partial E}{\partial V} - T\frac{\partial S}{\partial V} = \frac{\partial E}{\partial V} \ \ (= -P). \end{cases}$$

Thus

$$\begin{cases} \frac{\partial^2 F}{\partial T^2} = -\frac{\partial S}{\partial T} \\ \frac{\partial^2 F}{\partial V^2} = \frac{\partial^2 E}{\partial V \partial S}\frac{\partial S}{\partial V} + \frac{\partial^2 E}{\partial V^2}. \end{cases} \tag{17}$$

Next differentiate (16):

$$\begin{cases} 1 = \frac{\partial^2 E}{\partial S^2}\frac{\partial S}{\partial T} \\ 0 = \frac{\partial^2 E}{\partial S^2}\frac{\partial S}{\partial V} + \frac{\partial^2 E}{\partial S \partial V}. \end{cases}$$

Thus (17) gives:

$$\begin{cases} \frac{\partial^2 F}{\partial T^2} = -\left(\frac{\partial^2 E}{\partial S^2}\right)^{-1} \\ \frac{\partial^2 F}{\partial V^2} = \frac{\partial^2 E}{\partial V^2} - \left(\frac{\partial^2 E}{\partial S \partial V}\right)^2 \left(\frac{\partial^2 E}{\partial S^2}\right)^{-1}. \end{cases}$$

Since E is strictly convex:

$$\frac{\partial^2 E}{\partial S^2} > 0, \ \frac{\partial^2 E}{\partial V^2} > 0, \ \frac{\partial^2 E}{\partial S^2}\frac{\partial^2 E}{\partial V^2} > \left(\frac{\partial^2 E}{\partial S \partial V}\right)^2.$$

Hence:

$$\frac{\partial^2 F}{\partial T^2} < 0, \ \frac{\partial^2 F}{\partial V^2} > 0.$$

This proves (ii), and (iii),(iv) are similar. □

3. Maxwell's relations

Notation. We will hereafter regard T, P in some instances as independent variables (and not, as earlier, as functions of S, V). We will accordingly need better notation when we compute partial derivatives, to display which independent variables are involved. *The standard notation is to list the other independent variables outside parenthesis.*

For instance if we think of S as being a function of, say, T and V, we henceforth write

$$\left(\frac{\partial S}{\partial T}\right)_V$$

to denote the partial derivative of S in T, with V held constant, and

$$\left(\frac{\partial S}{\partial V}\right)_T$$

to denote the partial derivative of S in V, T constant. However *we will not employ parenthesis when computing the partial derivatives of E, F, G, H with respect to their "natural" arguments*. Thus if we are as usual thinking of F as a function of T, V, we write $\frac{\partial F}{\partial T}$, not $\left(\frac{\partial F}{\partial T}\right)_V$. □

We next compute the first derivatives of the thermodynamic potentials:

Energy. $E = E(S, V)$

$$\frac{\partial E}{\partial S} = T, \ \frac{\partial E}{\partial V} = -P. \tag{18}$$

Free energy. $F = F(T, V)$

$$\frac{\partial F}{\partial T} = -S, \ \frac{\partial F}{\partial V} = -P. \tag{19}$$

Enthalpy. $H = H(S, P)$

$$\frac{\partial H}{\partial S} = T, \ \frac{\partial H}{\partial P} = V. \tag{20}$$

Gibbs potential. $G = G(T, P)$

$$\frac{\partial G}{\partial T} = -S, \ \frac{\partial G}{\partial P} = V. \tag{21}$$

Proof. The formulas (18) simply record our definitions of T, P. The remaining identities are variants of the duality (3), (5). For instance, $F = E - TS$, where $T = \frac{\partial E}{\partial S}$, $S = S(T, V)$. So

$$\begin{aligned} \tfrac{\partial F}{\partial T} &= \tfrac{\partial E}{\partial S}\left(\tfrac{\partial S}{\partial T}\right)_V - S - T\left(\tfrac{\partial S}{\partial T}\right)_V \\ &= -S, \end{aligned}$$

as already noted earlier. □

We can now equate the mixed second partial derivatives of E, F, G, H to derive further identities. These are *Maxwell's relations*:

(22) $$\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial P}{\partial S}\right)_V$$

(23) $$\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V$$

(24) $$\left(\frac{\partial T}{\partial P}\right)_S = \left(\frac{\partial V}{\partial S}\right)_P$$

(25) $$\left(\frac{\partial S}{\partial P}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_P$$

The equality (22) just says $\frac{\partial^2 E}{\partial V \partial S} = \frac{\partial^2 E}{\partial S \partial V}$; (23) says $\frac{\partial^2 F}{\partial V \partial T} = \frac{\partial^2 F}{\partial T \partial V}$, etc.

E. Capacities

For later reference, we record here some notation:

(1) $$C_P = T\left(\frac{\partial S}{\partial T}\right)_P = \textit{ heat capacity at constant pressure}$$

(2) $$C_V = T\left(\frac{\partial S}{\partial T}\right)_V = \textit{ heat capacity at constant volume}$$

(3) $$\Lambda_P = T\left(\frac{\partial S}{\partial P}\right)_T = \textit{ latent heat with respect to pressure}$$

(4) $$\Lambda_V = T\left(\frac{\partial S}{\partial V}\right)_T = \textit{ latent heat with respect to volume}$$

(5) $$\beta = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P = \textit{ coefficient of thermal expansion}$$

(6) $$K_T = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T = \textit{ isothermal compressibility}$$

(7) $$K_S = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_S = \textit{ adiabatic compressibility.}$$

(See [B-S, p. 786-787] for the origin of the terms "latent heat", "heat capacity".)

There are many relationships among these quantities:

Lemma 4

(i) $C_V = \left(\frac{\partial E}{\partial T}\right)_V$
(ii) $C_P = \left(\frac{\partial H}{\partial T}\right)_P$
(iii) $C_P \geq C_V > 0$
(iv) $\Lambda_V - P = \left(\frac{\partial E}{\partial V}\right)_T$.

Proof. 1. Think of E as a function of T, V; that is, $E = E(S(T,V),V)$, where $S(T,V)$ means S as a function of T, V. Then

$$\left(\frac{\partial E}{\partial T}\right)_V = \frac{\partial E}{\partial S}\left(\frac{\partial S}{\partial T}\right)_V = T\left(\frac{\partial S}{\partial T}\right)_V = C_V.$$

Likewise, think of $H = H(S(T,P),P)$. Then

$$\left(\frac{\partial H}{\partial T}\right)_P = \frac{\partial H}{\partial S}\left(\frac{\partial S}{\partial T}\right)_P = T\left(\frac{\partial S}{\partial T}\right)_P = C_P,$$

where we used (20) from §D.

2. According to (19) in §D:

$$S = -\frac{\partial F}{\partial T}.$$

Thus

(8) $$C_V = T\left(\frac{\partial S}{\partial T}\right)_V = -T\frac{\partial^2 F}{\partial T^2} > 0,$$

since $T \mapsto F(T,V)$ is locally strictly concave. Likewise

$$S = -\frac{\partial G}{\partial T}$$

owing to (21) in §D; whence

(9) $$C_P = T\left(\frac{\partial S}{\partial T}\right)_P = -T\frac{\partial^2 G}{\partial T^2} > 0.$$

3. Now according to (12), (14) in §D:

$$G = F + PV;$$

that is,

$$\begin{cases} G(T,P) = F(T,V) + PV, \text{ where} \\ V = V(T,P) \text{ solves } \frac{\partial F}{\partial V}(T,V) = -P. \end{cases}$$

Consequently:

$$\begin{aligned} \tfrac{\partial G}{\partial T} &= \tfrac{\partial F}{\partial T} + \left(\tfrac{\partial F}{\partial V} + P\right)\left(\tfrac{\partial V}{\partial T}\right)_P \\ &= \tfrac{\partial F}{\partial T}, \end{aligned}$$

and so

$$\frac{\partial^2 G}{\partial T^2} = \frac{\partial^2 F}{\partial T^2} + \frac{\partial F}{\partial T \partial V}\left(\frac{\partial V}{\partial T}\right)_P. \tag{10}$$

But differentiating the identity $\partial F/\partial V(T,V) = -P$, we deduce

$$\frac{\partial^2 F}{\partial V \partial T} + \frac{\partial^2 F}{\partial V^2}\left(\frac{\partial V}{\partial T}\right)_P = 0.$$

Substituting into (10) and recalling (8), (9), we conclude

$$\begin{aligned} C_P - C_V &= T\left(\tfrac{\partial^2 F}{\partial T^2} - \tfrac{\partial^2 G}{\partial T^2}\right) \\ &= \tfrac{T}{\partial^2 F/\partial V^2}\left(\tfrac{\partial^2 F}{\partial V \partial T}\right)^2 \geq 0, \end{aligned} \tag{11}$$

since $V \mapsto F(T,V)$ is strictly convex.

This proves (iii). Assertion (iv) is left as an easy exercise. □

Remark. Using (19) in §D, we can write

$$C_P - C_V = -T\left(\frac{\partial P}{\partial T}\right)_V^2 \Big/ \left(\frac{\partial P}{\partial V}\right)_T \qquad \text{(Kelvin's formula)}. \tag{12}$$

□

F. More examples

1. Ideal gas

An *ideal gas* is a simple fluid with the equation of state

$$PV = RT, \tag{1}$$

where R is the gas constant (Appendix A) and we have normalized by taking $N = 1$ mole. As noted in §A, such an expression does *not* embody the full range of thermodynamic information available from the fundamental equation $S = S(E, V)$. We will see however that many conclusions can be had from (1) alone:

Theorem 1 *For an ideal gas,*

(i) C_P, C_V *are functions of* T *only:*

$$C_P = C_P(T),\ C_V = C_V(T).$$

(ii) $C_P - C_V = R$.

(iii) E *is a function of* T *only:*

$$E = E(T) = \int_{T_0}^{T} C_V(\theta)d\theta + E_0. \tag{2}$$

(iv) S *as a function of* (T, V) *is:*

$$S = S(T, V) = R\log V + \int_{T_0}^{T} \frac{C_V(\theta)}{\theta}d\theta + S_0. \tag{3}$$

Formulas (2), (3) characterize E, S up to additive constants.

Proof. 1. Since $E = E(S, V) = E(S(T, V), V)$, we have

$$\begin{aligned} \left(\tfrac{\partial E}{\partial V}\right)_T &= \tfrac{\partial E}{\partial S}\left(\tfrac{\partial S}{\partial V}\right)_T + \tfrac{\partial E}{\partial V} \\ &= T\left(\tfrac{\partial S}{\partial V}\right)_T - P \\ &= T\left(\tfrac{\partial P}{\partial T}\right)_V - P, \end{aligned}$$

where we utilized the Maxwell relation (23) in §D. But for an ideal gas, $T\left(\frac{\partial P}{\partial T}\right)_V - P = \frac{TR}{V} - P = 0$. Consequently $\left(\frac{\partial E}{\partial V}\right)_T = 0$. Hence if we regard E as a function of (T, V), E in fact depends only on T. But then, owing to the Lemma 4,

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V = \frac{dE}{dT}$$

depends only on T.

2. Next, we recall Kelvin's formula (12) in §E:

$$C_P - C_V = \frac{-T}{\left(\frac{\partial P}{\partial V}\right)_T}\left(\frac{\partial P}{\partial T}\right)_V^2.$$

Since $PV = RT$, we have

$$\begin{cases} \left(\frac{\partial P}{\partial V}\right)_T = -\frac{RT}{V^2}, \\ \left(\frac{\partial P}{\partial T}\right)_V = \frac{R}{V}. \end{cases}$$

Thus

$$C_P - C_V = \frac{T}{\left(\frac{RT}{V^2}\right)}\left(\frac{R^2}{V^2}\right) = R.$$

As R is constant and C_V depends only on T, C_P likewise depends only on T.

3. Finally, think of S as a function of T, V:

$$S = S(E(T,V),V) = S(E(T),V).$$

Then

$$\left(\frac{\partial S}{\partial T}\right)_V = \frac{\partial S}{\partial E}\frac{dE}{dT} = \frac{1}{T}C_V(T),$$

$$\left(\frac{\partial S}{\partial V}\right)_T = \frac{\partial S}{\partial V} = \frac{P}{T} = \frac{R}{V}.$$

Formula (3) follows. □

Remark. We can solve (2) for T as a function of E and so determine $S = S(T(E),V)$ as a function of (E,V). Let us check that

$$(E,V) \mapsto S \text{ is concave,}$$

provided

$$C_V > 0.$$

Now

$$\begin{cases} \frac{\partial S}{\partial E} &= \left(\frac{\partial S}{\partial T}\right)_V \frac{\partial T}{\partial E} = \frac{1}{T}C_V(T)\frac{1}{C_V(T)} = \frac{1}{T} \\ \frac{\partial S}{\partial V} &= \left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V = \frac{R}{V}. \end{cases}$$

Thus

$$\begin{cases} \frac{\partial^2 S}{\partial E^2} &= -\frac{1}{T^2}\frac{\partial T}{\partial E} = -\frac{1}{T^2 C_V(T)} < 0 \\ \frac{\partial^2 S}{\partial E \partial V} &= 0 \\ \frac{\partial^2 S}{\partial V^2} &= -\frac{R}{V^2} < 0, \end{cases}$$

and so $(E,V) \mapsto S$ is concave. □

Remark. Recalling §B, we can write for $N > 0$ moles of ideal gas:

$$PV = NRT, \tag{4}$$

and

$$\underbrace{S(E,V,N)}_{\substack{\text{The function } S \text{ of} \\ (E,V,N) \text{ from §B}}} = NS\left(\tfrac{E}{N}, \tfrac{V}{N}, 1\right)$$

$$= \underbrace{NS\left(\frac{E}{N}, \frac{V}{N}\right)}_{\text{The function } S \text{ of } (E,V) \text{ from §B.}}$$

We note next that

$$(E,V,N) \mapsto S \text{ is concave.} \tag{5}$$

Indeed if $0 < \lambda < 1$, $N, \hat{N} > 0$, then:

$$\begin{aligned}
&S(\lambda E + (1-\lambda)\hat{E}, \lambda V + (1-\lambda)\hat{V}, \lambda N + (1-\lambda)\hat{N}) \\
&= (\lambda N + (1-\lambda)\hat{N}) S\left(\tfrac{\lambda E + (1-\lambda)\hat{E}}{\lambda N + (1-\lambda)\hat{N}}, \tfrac{\lambda V + (1-\lambda)\hat{V}}{\lambda N + (1-\lambda)\hat{N}}\right) \\
&= (\lambda N + (1-\lambda)\hat{N}) S\left(\mu \tfrac{E}{N} + (1-\mu)\tfrac{\hat{E}}{\hat{N}}, \mu \tfrac{V}{N} + (1-\mu)\tfrac{\hat{V}}{\hat{N}}\right),
\end{aligned}$$

where

$$\mu = \frac{\lambda N}{\lambda N + (1-\lambda)\hat{N}}, 1 - \mu = \frac{(1-\lambda)\hat{N}}{\lambda N + (1-\lambda)\hat{N}}.$$

Since $(E,V) \mapsto S$ is concave, we deduce:

$$\begin{aligned}
&S(\lambda E + (1-\lambda)\hat{E}, \lambda V + (1-\lambda)\hat{V}, \lambda N + (1-\lambda)\hat{N}) \\
&\geq (\lambda N + (1-\lambda)\hat{N}) \left[\mu S\left(\tfrac{E}{N}, \tfrac{V}{N}\right) + (1-\mu) S\left(\tfrac{\hat{E}}{\hat{N}}, \tfrac{\hat{V}}{\hat{N}}\right)\right] \\
&= \lambda N S\left(\tfrac{E}{N}, \tfrac{V}{N}\right) + (1-\lambda)\hat{N} S\left(\tfrac{\hat{E}}{\hat{N}}, \tfrac{\hat{V}}{\hat{N}}\right) \\
&= \lambda S(E,V,N) + (1-\lambda) S(\hat{E}, \hat{V}, \hat{N}).
\end{aligned}$$

This proves (5). □

A *simple ideal gas* is an ideal gas for which C_V (and so C_P) are positive constants. Thus

$$\gamma := \frac{C_P}{C_V} > 1. \tag{6}$$

From (2), (3), we deduce for a simple ideal gas that

$$\begin{aligned}
E &= C_V T \\
S &= R \log V + C_V \log T + S_0
\end{aligned} \tag{7}$$

where we have set $E_0 = 0$. Thus for a *simple ideal gas*

$$\begin{aligned} &S(E,V) = R\log V + C_V \log E + S_0 \qquad (N=1) \\ &S(E,V,N) = NR\log\left(\tfrac{V}{N}\right) + NC_V \log\left(\tfrac{E}{N}\right) + S_0 N. \end{aligned} \tag{8}$$

(The constants S_0 in (7), (8) and below differ.) For later reference we record:

$$\begin{aligned} S &= C_V \log(TV^{\gamma-1}) + S_0 \\ S &= C_V \log(PV^{\gamma}) + S_0 \end{aligned} \tag{9}$$

where $\gamma = \frac{C_P}{C_V}$, $C_P - C_V = R$, $N = 1$.

2. Van der Waals fluid

A *van der Waals fluid* is a simple fluid with the equation of state

$$P = \frac{RT}{V-b} - \frac{a}{V^2} \qquad (V > b,\ N=1) \tag{10}$$

for constants $a, b > 0$.

Theorem 2 *For a van der Waals fluid,*

(i) C_V *is a function of* T *only:*

$$C_V = C_V(T).$$

(ii) E *as a function of* (T,V) *is:*

$$E = E(T,V) = \int_{T_0}^{T} C_V(\theta)d\theta - \frac{a}{V} + E_0. \tag{11}$$

(iii) S *as a function of* (T,V) *is*

$$S = S(T,V) = R\log(V-b) + \int_{T_0}^{T} \frac{C_V(\theta)}{\theta} d\theta + S_0. \tag{12}$$

Proof. 1. As in the previous proof,

$$\left(\frac{\partial E}{\partial V}\right)_T = T\left(\frac{\partial P}{\partial T}\right)_V - P.$$

But $P = \frac{RT}{V-b} - \frac{a}{V^2}$ and so $\left(\frac{\partial E}{\partial V}\right)_T = \frac{a}{V^2}$. Hence if we think of E as a function of (T,V), we deduce

$$E = -\frac{a}{V} + (\text{a function of } T \text{ alone}).$$

But then

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V$$

depends only on T. Formula (11) follows.

2. As before, $S = S(E(T,V),V)$. Then

$$\begin{array}{rcl} \left(\frac{\partial S}{\partial T}\right)_V & = & \frac{\partial S}{\partial E}\left(\frac{\partial E}{\partial T}\right)_V = \frac{1}{T}C_V(T), \\ \left(\frac{\partial S}{\partial V}\right)_T & = & \frac{\partial S}{\partial E}\left(\frac{\partial E}{\partial V}\right)_T + \frac{\partial S}{\partial V} \\ & = & \frac{1}{T}\frac{a}{V^2} + \frac{P}{T} \\ & = & \frac{R}{V-b}. \end{array}$$

Formula (12) results upon integration. □

Note. C_P depends on both T and V for a van der Waals fluid. □

We can define a *simple van der Waals fluid*, for which C_V is a constant. Then

$$\begin{cases} E = C_V T - \frac{a}{V} + E_0 \\ S = R\log(V-b) + C_V \log T + S_0, \end{cases} \qquad (N=1).$$

However if we solve for $S = S(E,V)$, S is *not concave everywhere*. Thus a van der Waals fluid fits into the foregoing framework only if we restrict attention to regions Σ where $(E,V) \mapsto S$ is concave.

Remark. More generally we can replace S by its *concave envelope* (= the smallest concave function greater than or equal to S in some region). See Callen [C] for a discussion of the physical meaning of all this. □

CHAPTER 2: Entropy and irreversibility

In Chapter I we began with an axiomatic model for a thermal system in equilibrium, and so could immediately discuss energy, entropy, temperature, etc. This point of view is static in time.

In this chapter we introduce various sorts of *processes*, involving changes in time of the parameters in what we now call a *thermodynamic system*. These, in conjunction with the *First and Second Laws* of thermodynamics, will allow us to *construct* E and S.

A. A model material

We begin by turning our attention again to the example of simple fluids, but now we reverse the point of view of Chapter I and ask rather: How can we construct the energy E and entropy S? We will follow Owen [O] (but see also Bharatha–Truesdell [B-T]).

1. Definitions

Since we intend to build E, S, we must start with other variables, which we take to be T, V.

A model for a homogeneous fluid body (without dissipation)

Assume we are given:

(a) an open, simply connected subset $\Sigma \subset (0,\infty) \times (0,\infty)$ (Σ is the *state space* and elements of Σ are called *states*)

and

(b) C^1-functions P, Λ_V, C_V defined on Σ (P is the *pressure*, Λ_V the *latent heat* with respect to volume, C_V the *heat capacity* at constant volume)

Notation. We write $P = P(T,V)$, $\Lambda_V = \Lambda_V(T,V)$, $C_V = C_V(T,V)$ to display the dependence of the functions P, Λ_V, C_V on (T,V). □

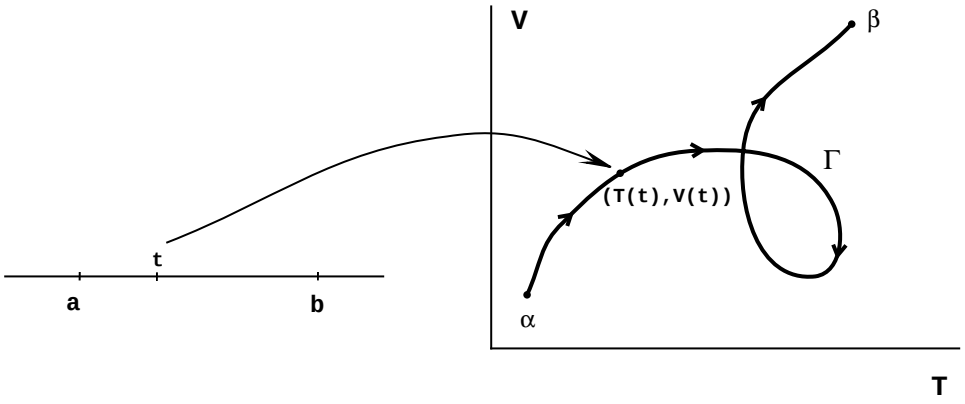
We further assume:

$$\frac{\partial P}{\partial V} < 0,\ \Lambda_V \neq 0,\ C_V > 0 \text{ in } \Sigma. \tag{1}$$

2. Energy and entropy

a. Working and heating

We define a *path* Γ for our model to be an oriented, continuous, piecewise C^1 curve in Σ. A path is a *cycle* if its starting and endpoints coincide.



Notation. We parameterize Γ by writing

$$\Gamma = \{(T(t), V(t)) \text{ for } a \le t \le b\},$$

where $a < b$ and $V, T : [a, b] \to \mathbb{R}$ are C^1. □

Definitions. (i) We define the *working* 1*-form*

$$đ W = P dV \tag{2}$$

and define the *work done by the fluid along* Γ to be

$$\mathbb{W}(\Gamma) = \int_\Gamma đ W = \int_\Gamma P dV. \tag{3}$$

(ii) We likewise define the *heating* 1*-form*

$$đ Q = C_V dT + \Lambda_V dV \tag{4}$$

and define the *net heat gained by the fluid along* Γ to be

$$\mathbb{Q}(\Gamma) = \int_\Gamma đ Q = \int_\Gamma C_V dT + \Lambda_V dV. \tag{5}$$

Remarks. (a) Thus

$$\mathbb{W}(\Gamma) = \int_a^b P(T(t), V(t))\dot{V}(t) dt \qquad \left(\dot{} = \frac{d}{dt}\right)$$

and

$$\mathbb{Q}(\Gamma) = \int_a^b C_V(T(t), V(t))\dot{T}(t) + \Lambda_V(T(t), V(t))\dot{V}(t)dt.$$

We call

$$w(t) = P(T(t), V(t))\dot{V}(t) \tag{6}$$

the *rate of working* and

$$q(t) = C_V(T(t), V(t))\dot{T}(t) + \Lambda_V(T(t), V(t))\dot{V}(t) \tag{7}$$

the *rate of heating* at time t $(a \leq t \leq b)$.

(b) Note very carefully that there *do not in general exist functions* W, Q of (T, V) whose differentials are the working, heating 1-forms. The slash through the "d" in $đW$, $đQ$ emphasizes this.

Consequently $\mathbb{W}(\Gamma)$, $\mathbb{Q}(\Gamma)$ *depend upon the path traversed by* Γ and not merely upon its endpoints. However, $\mathbb{W}(\Gamma)$, $\mathbb{Q}(\Gamma)$ do not depend upon the parameterizations of Γ. □

Physical interpretations. (1) If we think of our homogeneous fluid body as occupying the region $U(t) \subset \mathbb{R}^3$ at time t, then the rate of work at time t is

$$w(t) = \int_{\partial U(t)} P\mathbf{v} \cdot \boldsymbol{\nu}\ dS,$$

$\mathbf{v}$ denoting the velocity field and $\boldsymbol{\nu}$ the outward unit normal field along $\partial U(t)$. Since we assume P is independent of position, we have

$$\begin{aligned} w(t) = P\textstyle\int_{\partial U(t)} \mathbf{v} \cdot \boldsymbol{\nu} dS &= P\frac{d}{dt}\left(\int_{U(t)} dx\right) \\ &= P\dot{V}(t), \end{aligned}$$

in accordance with (6).

(2) Similarly, Λ_V records the gain of heat owing to the volume change (at fixed temperature T) and C_V records the gain of heat due to temperature change (at fixed volume V). □

Definitions. Let $\Gamma = \{(T(t), V(t)) \mid a \leq t \leq b\}$ be a path in Σ.

(i) Γ is called *isothermal* if $T(t)$ is constant $(a \leq t \leq b)$.

(ii) Γ is called *adiabatic* if $q(t) = 0$ $(a \leq t \leq b)$.

Construction of adiabatic paths. Since $q(t) = C_V(T(t), V(t))\dot{T}(t) + \Lambda_V(T(t), V(t))\dot{V}(t)$, $(a \leq t \leq b)$, we can construct adiabatic paths by introducing the parameterization $(T, V(T))$ and solving the ODE

$$\frac{dV}{dT} = -\frac{C_V(V, T)}{\Lambda_V(V, T)} \qquad \textit{ODE for adiabatic paths} \tag{8}$$

for V as a function of T, $V = V(T)$. Taking different initial conditions for (8) gives different adiabatic paths (a.k.a. adiabats).

Any C^1 parameterization of the graph of $V = V(T)$ gives an adiabatic path.

b. The First Law, existence of E

We turn now to our basic task, building E, S for our fluid system. The existence of these quantities will result from physical principles, namely the First and Second Laws of thermodynamics.

We begin with a form of the *First Law*: We hereafter assume that for every *cycle* Γ of our homogeneous fluid body, we have:

$$\mathbb{W}(\Gamma) = \mathbb{Q}(\Gamma). \tag{9}$$

This is *conservation of energy*: The work done by the fluid along any cycle equals the heat gained by the fluid along the cycle.

Remark. We assume in (9) that the units of work and heat are the same. If not, e.g. if heat is measured in calories and work in Joules (Appendix A), we must include in (9) a multiplicative factor on the right hand side called the *mechanical equivalent of heat* (= 4.184J/calorie).

□

We deduce this immediate mathematical corollary:

Theorem 1 *For our homogeneous fluid body, there exists a C^2 function $E : \Sigma \to \mathbb{R}$ such that*

$$\frac{\partial E}{\partial V} = \Lambda_V - P, \ \frac{\partial E}{\partial T} = C_V. \tag{10}$$

We call $E = E(T, V)$ the *internal energy.*

Proof. According to (3), (5), (9):

$$\int_\Gamma C_V dT + (\Lambda_V - P)dV = 0$$

for each cycle in Σ. The 1-form $C_V dT + (\Lambda_V - P)dV$ is thus exact, since Σ is open, simply connected. This means there exists a C^2 function E with

$$dE = C_V dT + (\Lambda_V - P)dV. \tag{11}$$

This statement is the same as (10). □

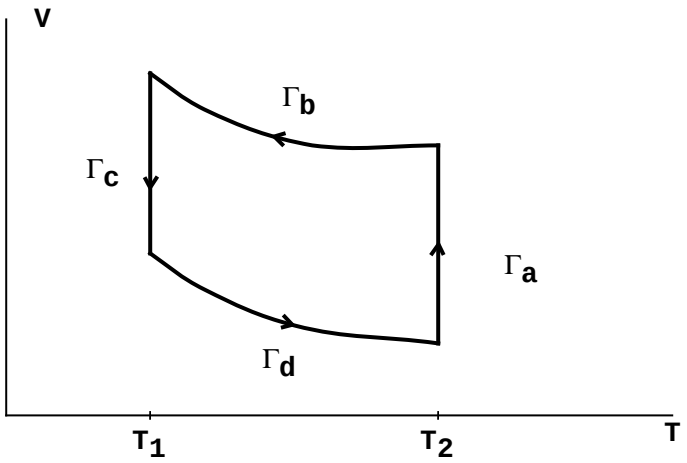
Notation. From (11), it follows that

$$dE = đQ - đW \tag{12}$$

exact 1-form; non-exact 1-forms

c. Carnot cycles

Definition. A *Carnot cycle* Γ for our fluid is a cycle consisting of two distinct adiabatic paths and two distinct isothermal paths, as drawn:



(We assume $\Lambda_V > 0$ for this picture and take a counterclockwise orientation.)

We have $\mathbb{Q}(\Gamma_b) = \mathbb{Q}(\Gamma_d) = 0$, since Γ_b, Γ_d are adiabatic paths.

Notation.

$$\begin{aligned} \mathbb{Q}^- &= -\mathbb{Q}(\Gamma_c) = \textit{heat emitted at temperature } T_1 \\ \mathbb{Q}^+ &= \mathbb{Q}(\Gamma_a) = \textit{heat gained at temperature } T_2 \\ \mathbb{Q} &= \mathbb{W}(\Gamma) = \mathbb{Q}^+ - \mathbb{Q}^- = \textit{work.} \end{aligned}$$

Definition. A Carnot cycle Γ is a *Carnot heat engine* if

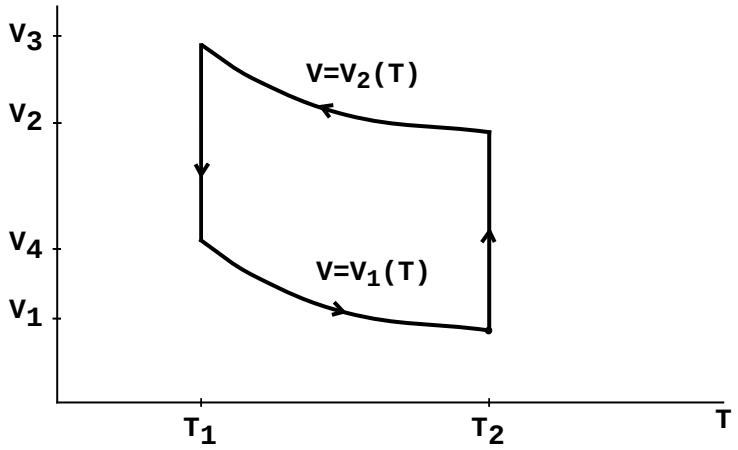
$$\underbrace{\mathbb{Q}^+ > 0}_{\text{heat is gained at the higher temperature } T_2} \quad \text{and} \quad \underbrace{\mathbb{Q}^- > 0}_{\text{heat is lost at the lower temperature } T_1} \tag{13}$$

The picture above illustrates the correct orientation of Γ for a Carnot heat engine, provided $\Lambda_V > 0$.

Example. Suppose our fluid body is in fact an *ideal gas* (discussed in §I.F). Then $PV = RT$ if we consider $N = 1$ mole, and

$$\left\{ \begin{array}{rcl} P(T,V) & = & \frac{RT}{V},\ C_V(T,V) = C_V(T), \\ \Lambda_V(T,V) & = & \frac{RT}{V}. \end{array} \right. \tag{14}$$

(The formula for Λ_V is motivated by our recalling from §I.E that we should have $\Lambda_V = T\left(\frac{\partial S}{\partial V}\right)_T = T\left(\frac{\partial P}{\partial T}\right)_V = \frac{RT}{V}$.) Consider a Carnot heat engine, as drawn:



We compute

$$\mathbb{Q}^+ = \int_{V_1}^{V_2} \Lambda_V dV = RT_2 \log\left(\frac{V_2}{V_1}\right). \tag{15}$$

The equation for the adiabatic parts of the cycle, according to (8), is:

$$\frac{dV}{dT} = -\frac{C_V}{\Lambda_V} = -\frac{VC_V(T)}{RT}.$$

Hence the formulas for the lower and upper adiabats are:

$$\left\{ \begin{array}{rcl} V_1(T) & = & V_1 \exp\left(-\int_{T_2}^{T} \frac{C_V(\theta)}{R\theta} d\theta\right) \\ V_2(T) & = & V_2 \exp\left(-\int_{T_2}^{T} \frac{C_V(\theta)}{R\theta} d\theta\right), \end{array} \right.$$

and so

$$\left\{ \begin{array}{rcl} V_4 & = & V_1(T_1) = V_1 \exp\left(-\int_{T_2}^{T_1} \frac{C_V(\theta)}{R\theta} d\theta\right) \\ V_3 & = & V_2(T_1) = V_2 \exp\left(-\int_{T_2}^{T_1} \frac{C_V(\theta)}{R\theta} d\theta\right). \end{array} \right.$$

Therefore

$$\begin{aligned}\mathbb{Q}^- = -\int_{V_3}^{V_4} \Lambda_V dV &= -RT_1 \log\left(\tfrac{V_4}{V_3}\right) \\ &= -RT_1 \log\left(\tfrac{V_1}{V_2}\right) > 0.\end{aligned}$$

The work is

$$\begin{aligned}\mathbb{W} &= \mathbb{Q}^+ - \mathbb{Q}^- \\ &= R(T_2 - T_1)\log\left(\tfrac{V_2}{V_1}\right) \\ &> 0;\end{aligned}$$

and for later reference we deduce from (15) that

$$\mathbb{W} = \left(1 - \frac{T_1}{T_2}\right)\mathbb{Q}^+ \qquad \text{for a } \textit{Carnot cycle of an ideal gas.} \tag{16}$$

□

d. The Second Law

We next hypothesize the following form of the *Second Law* of thermodynamics: For each Carnot heat engine Γ of our homogeneous fluid body, operating between temperatures $T_1 < T_2$, we have

$$\mathbb{W} > 0$$

and

$$\mathbb{W} = \left(1 - \frac{T_1}{T_2}\right)\mathbb{Q}^+. \tag{17}$$

In other words we are *assuming* that formula (17), which we showed above holds for any Carnot heat engine for an ideal gas, in fact holds for any Carnot heat engine for our general homogeneous fluid body.

Physical interpretation. The precise relation (17) can be motivated as follows from this general, if vague, statement, due essentially to Clausius:

$$\left\{\begin{array}{l}\text{“no system which employs homogeneous fluid bodies} \\ \text{operating through cycles can absorb heat at one temperature} \\ T_1 \text{ and emit the same amount of heat at a higher} \\ \text{temperature } T_2 > T_1, \text{ without doing work on its environment”}.\end{array}\right. \tag{18}$$

Let us first argue physically that (18) implies this assertion:

$$\left\{\begin{array}{l}\text{“If } \Gamma, \tilde{\Gamma} \text{ are two Carnot heat engines (for possibly} \\ \text{different homogeneous fluid bodies) and } \Gamma, \tilde{\Gamma} \text{ both operate} \\ \text{between the same temperatures } T_2 > T_1, \text{ then} \\ \qquad \mathbb{W} = \tilde{\mathbb{W}} \text{ implies } \mathbb{Q}^+ = \tilde{\mathbb{Q}}^+.\text{”}\end{array}\right. \tag{19}$$

This says that "any two Carnot cycles which operate between the same temperatures and which perform the same work, must absorb the same heat at the higher temperature".

Physical derivation of (19) from (18). To see why (19) is in some sense a consequence of (18), suppose not. Then for two fluid bodies we could find Carnot heat engines $\Gamma, \tilde{\Gamma}$ operating between the temperatures $T_2 > T_1$, such that

$$\mathbb{W} = \tilde{\mathbb{W}}, \text{ but } \mathbb{Q}^+ > \tilde{\mathbb{Q}}^+.$$

Then since $\mathbb{W} = \tilde{\mathbb{W}}$, we observe

$$(\tilde{\mathbb{Q}}^- - \mathbb{Q}^-) = \tilde{\mathbb{Q}}^+ - \mathbb{Q}^+ < 0.$$

Imagine now the process Δ consisting of "$\tilde{\Gamma}$ followed by the reversal of Γ". Then Δ would *absorb* $\mathbb{Q} = -(\tilde{\mathbb{Q}}^- - \mathbb{Q}^-) > 0$ units of heat at the lower temperature T_1 and *emit* the same $\mathbb{Q}$ units of heat at the higher temperature. But since $\tilde{\mathbb{W}} - \mathbb{W} = 0$, no work would be performed by Δ. This would all contradict (18), however.

Physical derivation of (17) from (19). Another way of stating (19) is that for a Carnot heat engine, $\mathbb{Q}^+$ is some function $\phi(T_1, T_2, \mathbb{W})$ of the operating temperatures T_1, T_2 and the work $\mathbb{W}$, and further *this function ϕ is the same for all fluid bodies.*

But (16) says

$$\mathbb{Q}^+ = \frac{T_2}{T_2 - T_1}\mathbb{W} = \phi(T_1, T_2, \mathbb{W})$$

for an ideal gas. Hence (19) implies we have the same formula for any homogeneous fluid body. This is (17). □

Remark. See Owen [O], Truesdell [TR, Appendix 1A], Bharatha–Truesdell [B-T] for a more coherent discussion. □

e. Existence of S

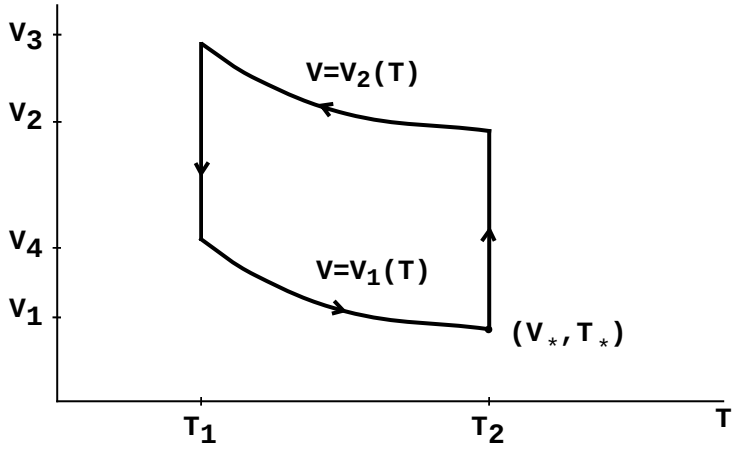
We next exploit (17) to build an entropy function S for our model homogeneous fluid body:

Theorem 2 *For our homogeneous fluid body, there exists a C^2 function $S : \Sigma \to \mathbb{R}$ such that*

$$\frac{\partial S}{\partial V} = \frac{\Lambda_V}{T}, \ \frac{\partial S}{\partial T} = \frac{C_V}{T}. \tag{20}$$

We call $S = S(T, V)$ the *entropy.*

Proof. 1. Fix a point (T_*, V_*) in Σ and consider a Carnot heat engine as drawn (assuming $\Lambda_V > 0$):



Now

$$\mathbb{Q}^+ = \int_{V_1}^{V_2} \Lambda_V(V, T_2) dV. \tag{21}$$

Furthermore

$$\mathbb{W} = \int_\Gamma P dV = \int_{T_1}^{T_2} \int_{V_1(T)}^{V_2(T)} \frac{\partial P}{\partial T} dV \; dT$$

by the Gauss–Green Theorem. This identity, (17) and (21) imply

$$\int_{V_1}^{V_2} \Lambda_V(V, T_2) dV = \frac{T_2}{T_2 - T_1} \int_{T_1}^{T_2} \int_{V_1(T)}^{V_2(T)} \frac{\partial P}{\partial T} dV dT.$$

Let $T_1 \to T_2 = T_*$:

$$\int_{V_1}^{V_2} \Lambda_V(V, T_*) dV = T_* \int_{V_1}^{V_2} \frac{\partial P}{\partial T}(V, T_*) dV.$$

Divide by $V_2 - V_1$ and let $V_2 \to V_1 = V_*$, to deduce

$$\Lambda_V = T \frac{\partial P}{\partial T} \qquad \text{(Clapeyron's formula)} \tag{22}$$

at the point (T_*, V_*). Since this point was arbitrary, the identity (22) is valid everywhere in Σ.

2. Recall from (10) that

$$\frac{\partial E}{\partial V} = \Lambda_V - P, \; \frac{\partial E}{\partial T} = C_V. \tag{23}$$

Consequently:

$$\begin{aligned}\tfrac{\partial}{\partial T}\left(\tfrac{\Lambda_V}{T}\right) &= \tfrac{1}{T}\tfrac{\partial \Lambda_V}{\partial T} - \tfrac{\Lambda_V}{T^2} \\ &= \tfrac{1}{T}\left(\tfrac{\partial^2 E}{\partial V \partial T} + \tfrac{\partial P}{\partial T}\right) - \tfrac{1}{T}\left(\tfrac{\partial P}{\partial T}\right) \text{ by (22), (23)} \\ &= \tfrac{\partial}{\partial V}\left(\tfrac{C_V}{T}\right) \text{ by (23) again.}\end{aligned}$$

Thus the form

$$\frac{C_V}{T}dT + \frac{\Lambda_V}{T}dV$$

is exact: there exists a C^2-function S such that

$$dS = \frac{C_V}{T}dT + \frac{\Lambda_V}{T}dV. \tag{24}$$

This is (20). □

Notation. From (24) it follows that

$$dS = \frac{đ\, Q}{T}, \tag{25}$$

and so (12) becomes Gibbs' formula:

$$dE = TdS - PdV.$$

S **as a function of** (E, V). We have determined E, S as functions of (T, V). To be consistent with the axiomatic approach in Chapter I, however, we *should consider* S *as a function of the extensive variables* (E, V).

First, since $\frac{\partial E}{\partial T} = C_V > 0$, we can solve for $T = T(E, V)$. Then $P = P(T, V) = P(T(E, V), V)$ gives P as a function of (E, V). Also the formulas $S = S(T, V) = S(T(E, V), V)$ display S as a function of (E, V). Consequently

$$\begin{aligned}\left(\tfrac{\partial S}{\partial E}\right)_V &= \left(\tfrac{\partial S}{\partial T}\right)_V \tfrac{\partial T}{\partial E} \\ &= \tfrac{C_V}{T}\tfrac{1}{C_V} = \tfrac{1}{T} \text{ by (20)}\end{aligned} \tag{26}$$

and

$$\begin{aligned}\left(\tfrac{\partial S}{\partial V}\right)_E &= \left(\tfrac{\partial S}{\partial T}\right)_V \tfrac{\partial T}{\partial V} + \left(\tfrac{\partial S}{\partial V}\right)_T \\ &= \tfrac{C_V}{T}\tfrac{\partial T}{\partial V} + \tfrac{\Lambda_V}{T} \text{ by (20).}\end{aligned} \tag{27}$$

But $E(T(W, V), V) = W$ for all W and so

$$\left(\frac{\partial E}{\partial T}\right)_V \frac{\partial T}{\partial V} + \left(\frac{\partial E}{\partial V}\right)_T = 0.$$

Hence (10) implies

$$C_V \frac{\partial T}{\partial V} = P - \Lambda_V. \tag{28}$$

Consequently (27) says $\left(\frac{\partial S}{\partial V}\right)_E = \frac{P}{T}$. In summary:

$$\left(\frac{\partial S}{\partial E}\right)_V = \frac{1}{T},\ \left(\frac{\partial S}{\partial V}\right)_E = \frac{P}{T}, \tag{29}$$

as expected from the general theory in Chapter I.

Finally we check that

$$S \textit{ is a concave function of } (E, V). \tag{30}$$

For proving this, we deduce first from (29) that for $S = S(E, V)$:

$$\frac{\partial^2 S}{\partial E^2} = -\frac{1}{C_V T^2} < 0. \tag{31}$$

Also

$$\frac{\partial^2 S}{\partial V^2} = \frac{\left(\frac{\partial P}{\partial V}\right)_E}{T} - \frac{P\left(\frac{\partial T}{\partial V}\right)_E}{T^2}.$$

Now

$$\left(\frac{\partial P}{\partial V}\right)_E = \frac{\partial P}{\partial V} + \frac{\partial P}{\partial T}\left(\frac{\partial T}{\partial V}\right)_E,$$

and so

$$\frac{\partial^2 S}{\partial V^2} = \frac{1}{T}\frac{\partial P}{\partial V} + \frac{1}{T^2}\left[T\frac{\partial P}{\partial T} - P\right]\left(\frac{\partial T}{\partial V}\right)_E.$$

But

$$\left(\frac{\partial T}{\partial V}\right)_E = \frac{-\frac{\partial E}{\partial V}}{\frac{\partial E}{\partial T}} = \frac{P - \Lambda_V}{C_V} \text{ by (10)},$$

and (22) says:

$$\Lambda_V = T\frac{\partial P}{\partial T}.$$

Thus

$$\frac{\partial^2 S}{\partial V^2} = \frac{1}{T}\frac{\partial P}{\partial V} - \frac{1}{C_V T^2}(P - \Lambda_V)^2 < 0, \tag{32}$$

since $\frac{\partial P}{\partial V} < 0$, $C_V > 0$. Lastly,

$$\frac{\partial^2 S}{\partial E \partial V} = \frac{-\left(\frac{\partial T}{\partial V}\right)_E}{T^2} = \frac{\Lambda_V - P}{T^2 C_V}.$$

Consequently (31), (32) imply

$$
\begin{aligned}
&\left(\tfrac{\partial^2 S}{\partial E^2}\right)\left(\tfrac{\partial^2 S}{\partial V^2}\right) - \left(\tfrac{\partial^2 S}{\partial E \partial V}\right)^2 \\
&= \left(-\tfrac{1}{C_V T^2}\right)\left(\tfrac{1}{T}\tfrac{\partial P}{\partial V} - \tfrac{1}{C_V T^2}(P-\Lambda_V)^2\right) \\
&-\tfrac{(\Lambda_V - P)^2}{T^4 C_V^2} > 0.
\end{aligned} \tag{33}
$$

Owing to (31), (32), (33) S is a concave function of (E, V). □

3. Efficiency of cycles

Recall from §2 that

$$
\begin{aligned}
q(t) &= \text{rate of heating at time } t \\
&= C_V(T(t), V(t))\dot{T}(t) + \Lambda_V(T(t), V(t))\dot{V}(t),
\end{aligned}
$$

where $\Gamma = \{(T(t), V(t)) \mid a \le t \le b\}$ is a path in Σ.

Notation.

(i)

$$
\begin{aligned}
q^+(t) &= \begin{cases} q(t) & \text{if } q(t) \ge 0 \\ 0 & \text{if } q(t) \le 0 \end{cases} \\
q^-(t) &= \begin{cases} 0 & \text{if } q(t) \ge 0 \\ -q(t) & \text{if } q(t) \le 0 \end{cases} \\
q(t) &= q^+(t) - q^-(t) \quad (a \le t \le b)
\end{aligned}
$$

(ii)

$$
\begin{aligned}
\mathbb{Q}^+(\Gamma) &= \int_a^b q^+(t)dt = \textit{heat gained along } \Gamma \\
\mathbb{Q}^-(\Gamma) &= \int_a^b q^-(t)dt = \textit{heat emitted along } \Gamma
\end{aligned}
$$

(iii)

$$
\mathbb{W}(\Gamma) = \mathbb{Q}^+(\Gamma) - \mathbb{Q}^-(\Gamma) = \textit{work performed along } \Gamma.
$$

Definition. Assume Γ is a cycle. The *efficiency* of Γ is

$$
\eta = \frac{\mathbb{W}(\Gamma)}{\mathbb{Q}^+(\Gamma)}, \tag{34}
$$

the ratio of the work performed to the heat absorbed. Note $0 \le \eta \le 1$.

Example. If Γ is a Carnot heat engine operating between temperatures $0 < T_1 < T_2$, we have

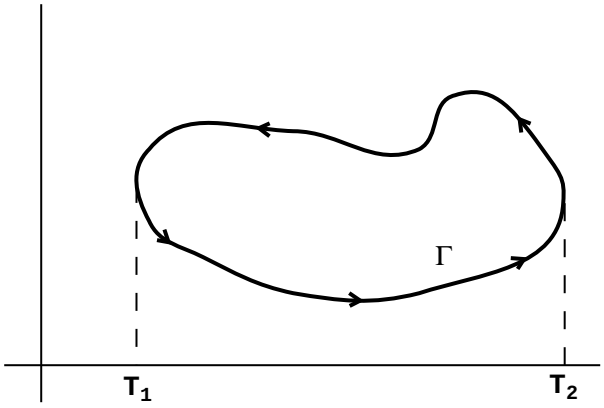
$$\eta = 1 - \frac{T_1}{T_2} \tag{35}$$

according to (16). □

Notation. Let Γ be an arbitrary cycle in Σ, with parameterization $\{(T(t), V(t)) \mid a \leq t \leq b\}$. Let

$$\begin{cases} T_1 &= \min\{T(t) \mid a \leq t \leq b\} \\ T_2 &= \max\{T(t) \mid a \leq t \leq b\} \end{cases} \tag{36}$$

denote the highest and lowest temperatures occurring in the cycle.



Theorem 3 *Let Γ be a cycle as above, and let η denote its efficiency. Then*

$$\eta \leq 1 - \frac{T_1}{T_2}. \tag{37}$$

Proof. According to (20),

$$\frac{q}{T} = \frac{C_V}{T}\dot{T} + \frac{\Lambda_V}{T}\dot{V} = \frac{d}{dt}S(T(t), V(t)).$$

Since Γ is a cycle, we therefore have

$$0 = \int_\Gamma \frac{đ Q}{T} = \int_a^b \frac{q}{T} dt. \tag{38}$$

Then

$$
\begin{aligned}
0 &= \int_a^b \frac{q^+}{T} - \frac{q^-}{T} dt \\
&\geq \frac{1}{T_2}\int_a^b q^+ dt - \frac{1}{T_1}\int_a^b q^- dt, \\
&= \frac{\mathbb{Q}^+(\Gamma)}{T_2} - \frac{\mathbb{Q}^-(\Gamma)}{T_1}
\end{aligned} \tag{39}
$$

since $q^+ \geq 0$, $q^- \geq 0$, $T_1 \leq T \leq T_2$ on Γ.

Consequently:

$$
\begin{aligned}
\eta = \frac{\mathbb{W}(\Gamma)}{\mathbb{Q}^+(\Gamma)} &= 1 - \frac{\mathbb{Q}^-(\Gamma)}{\mathbb{Q}^+(\Gamma)} \\
&\leq 1 - \frac{T_1}{T_2}.
\end{aligned}
$$

□

We will later (in §B) take the efficiency estimate (37) as a starting point for more general theory.

4. Adding dissipation, Clausius inequality

We propose next, following Owen [O] and Serrin [S1], to modify our model to include irreversible, dissipative effects.

Notation. Remember that we represent a parametric curve Γ by writing

$$(T(t), V(t)) \text{ for } a \leq t \leq b, \tag{40}$$

where $a < b$ and $V, T : [a, b] \to \mathbb{R}$ are C^1. We will henceforth call Γ a *process* to emphasize that the following constructions depend on the parameterization. We call Γ a *cyclic process* if $(T(a), V(a)) = (T(b), V(b))$.

A model for a homogeneous fluid body (with dissipation). Assume we are given:

(a) a convex open subset $\Sigma \subset (0, \infty) \times (0, \infty)$ (Σ is the *state space*),

and

(b) two C^2 functions $\mathcal{W}, \mathcal{Q}$ defined on $\Sigma \times \mathbb{R}^2$.

Notation. We will write

$$
\begin{aligned}
\mathcal{W} &= \mathcal{W}(T, V, A, B) \\
\mathcal{Q} &= \mathcal{Q}(T, V, A, B)
\end{aligned}
$$

where $(T, V) \in \Sigma$, $(A, B) \in \mathbb{R}^2$. □

We assume further that $\mathcal{W}, \mathcal{Q}$ have the form:

$$
\begin{aligned}
\mathcal{W}(T, V, A, B) &= P(T, V)B + R_1(T, V, A, B) \\
\mathcal{Q}(T, V, A, B) &= C_V(T, V)A + \Lambda_V(T, V)B + R_2(T, V, A, B)
\end{aligned} \tag{41}
$$

for all $(T,V) \in \Sigma$, $(A,B) \in \mathbb{R}^2$, where the *remainder terms* R_1, R_2 satisfy:

$$|R_1(T,V,A,B), R_2(T,V,A,B)| \leq C(A^2+B^2) \tag{42}$$

for some constant C and all $(T,V),(A,B)$ as above. Lastly we suppose that P, C_V, Λ_V satisfy:

$$\frac{\partial P}{\partial V} < 0,\ \Lambda_V \neq 0,\ C_V > 0 \text{ in } \Sigma. \tag{43}$$

Given a process Γ as above, we define the *work done by the fluid along* Γ to be

$$\mathbb{W}(\Gamma) = \int_\Gamma đ W = \int_a^b \mathcal{W}(T(t),V(t),\dot{T}(t),\dot{V}(t))dt \tag{44}$$

and the *net heat gained by the fluid along* Γ to be

$$\mathbb{Q}(\Gamma) = \int_\Gamma đ Q = \int_a^b \mathcal{Q}(T(t),V(t),\dot{T}(t),\dot{V}(t))dt. \tag{45}$$

Notation. We call

$$w(t) = \mathcal{W}(T(t),V(t),\dot{T}(t),\dot{V}(t)) \tag{46}$$

the rate of working and

$$q(t) = \mathcal{Q}(T(t),V(t),\dot{T}(t),\dot{V}(t)) \qquad (a \leq t \leq b) \tag{47}$$

the *rate of heating* at time t. In this model the expressions "$\int_\Gamma đ W$" and "$\int_\Gamma đ Q$" are defined by (44), (45), but "$đ W$" and "$đ Q$" are not defined.

Remark. Note very carefully: $\mathbb{W}(\Gamma), \mathbb{Q}(\Gamma)$ depend not only on the path described by Γ but also on the parameterization. □

Our intention is to build energy and entropy functions for our new model fluid with dissipation. As before we start with a form of the First Law: For each cyclic process Γ of our homogeneous fluid body with dissipation, we assume

$$\mathbb{W}(\Gamma) = \mathbb{Q}(\Gamma). \tag{48}$$

This is again conservation of energy, now hypothesized for every cyclic process, i.e. for each cycle as a path and each parameterization.

Theorem 4 *There exists a C^2 function $E : \Sigma \to \mathbb{R}$ such that*

$$\frac{\partial E}{\partial T} = C_V,\ \frac{\partial E}{\partial V} = \Lambda_V - P. \tag{49}$$

Proof. Consider any cyclic process Γ.

We may assume $a = 0$, $b > 0$. Then (48) says

$$\int_0^b \mathcal{W}(T(t), V(t), \dot{T}(t), \dot{V}(t))dt = \int_0^b \mathcal{Q}(T(t), V(t), \dot{T}(t), \dot{V}(t))dt.$$

Owing to (41), we can rewrite:

$$\int_0^b C_V \dot{T} + (\Lambda_V - P)\dot{V}dt = \int_0^b R_1(T, V, \dot{T}, \dot{V}) - R_2(T, V, \dot{T}, \dot{V})dt.$$

This identity must hold for each parameterization. So fix $\varepsilon > 0$ and set

$$(T_\varepsilon(t), V_\varepsilon(t)) = (T(\varepsilon t), V(\varepsilon t)) \quad (0 \le t \le b/\varepsilon).$$

Then

$$\int_0^{b/\varepsilon} C_V \dot{T}_\varepsilon + (\Lambda_V - P)\dot{V}_\varepsilon dt = \int_0^{b/\varepsilon} R_1(T_\varepsilon, V_\varepsilon, \dot{T}_\varepsilon, \dot{V}_\varepsilon) - R_2(T_\varepsilon, V_\varepsilon, \dot{T}_\varepsilon, \dot{V}_\varepsilon)dt. \tag{50}$$

Since $\dot{T}_\varepsilon(t) = \varepsilon \dot{T}(\varepsilon t)$, $\dot{V}_\varepsilon(t) = \varepsilon \dot{V}(\varepsilon t)$, we can rewrite the left hand side of (51) as

$$\int_0^b C_V \dot{T} + (\Lambda_V - P)\dot{V}dt = \int_\Gamma C_V dT + (\Lambda_V - P)dV, \tag{51}$$

where we use 1-form notation to emphasize that this term does not depend on the parameterization. However (42) implies

$$\begin{aligned} &\left| \textstyle\int_0^{b/\varepsilon} R_1(T_\varepsilon, V_\varepsilon, \dot{T}_\varepsilon, \dot{V}_\varepsilon) - R_2(T_\varepsilon, V_\varepsilon, \dot{T}_\varepsilon, \dot{V}_\varepsilon)dt \right| \\ &\le C\tfrac{b}{\varepsilon} \max_{0 \le t \le b/\varepsilon}[(\dot{T}_\varepsilon)^2 + (\dot{V}_\varepsilon)^2] \\ &\le C\varepsilon. \end{aligned}$$

Sending $\varepsilon \to 0$, we conclude

$$\int_\Gamma C_V dT + (\Lambda_V - P)dV = 0$$

for each cycle Γ in Σ, and the existence of E follows. □

Remark. In fact (48) implies

$$R_1(T, V, A, B) = R_2(T, V, A, B) \tag{52}$$

for all $(T,V) \in \Sigma$, $(A,B) \in \mathbb{R}^2$. To see this, consider any process Γ parameterized by $(T(t),V(t))$, where $a \le t \le 0$. Extend Γ to a *cyclic* process Δ parameterized by $(T(t),V(t))$ for $a \le t \le 1$. Then by the proof above:

$$\int_a^1 R_1(T,V,\dot{T},\dot{V})dt = \int_a^1 R_2(T,V,\dot{T},\dot{V})dt. \tag{53}$$

Reparameterize by writing

$$\begin{aligned} T_\varepsilon(t) &= \begin{cases} T(t) & a \le t \le 0 \\ T(\varepsilon t) & 0 \le t \le 1/\varepsilon, \end{cases} \\ V_\varepsilon(t) &= \begin{cases} V(t) & a \le t \le 0 \\ V(\varepsilon t) & 0 \le t \le 1/\varepsilon. \end{cases} \end{aligned}$$

Formula (53) holds for any parameterization and so is valid with $(T_\varepsilon, V_\varepsilon, \dot{T}_\varepsilon, \dot{V}_\varepsilon)$ replacing $(T,V,\dot{T},\dot{V})$. Making this change and letting $\varepsilon \to 0$, we deduce

$$\int_a^0 R_1(T,V,\dot{T},\dot{V})dt = \int_a^0 R_2(T,V,\dot{T},\dot{V})dt$$

for any process $(T(t),V(t))$, $a \le t \le 0$. This is only possible if $R_1 \equiv R_2$. □

The foregoing proofs demonstrate that our model with dissipation in some sense "approximates an ideal model without dissipation" in the limit as we consider our processes on "slower and slower time scales". The model without dissipation corresponds simply to setting $R_1 \equiv 0$, $R_2 \equiv 0$.

To further develop our model we next assume as an instance of the Second Law that

$$\mathbb{W} > 0$$

and

$$\mathbb{W} = \left(1 - \frac{T_1}{T_2}\right) \mathbb{Q}^+ \tag{54}$$

for any Carnot heat engine of the ideal model without dissipation acting between temperatures $T_2 > T$. This assertion as before implies there exists a C^2 function $S : \Sigma \to \mathbb{R}$ with

$$\frac{\partial S}{\partial T} = \frac{C_V}{T}, \ \frac{\partial S}{\partial V} = \frac{\Lambda_V}{T}. \tag{55}$$

Finally it seems reasonable to assume

$$R_1(T,V,A,B) = R_2(T,V,A,B) \le 0 \tag{56}$$

for all $(T, V) \in \Sigma$, $(A, B) \in \mathbb{R}^2$. Indeed we can interpret for any process Γ the term

$$\int_a^b R_1(T, V, \dot{T}, \dot{V})dt$$

as representing the *lost* amount of work performed by the fluid along Γ owing to velocity dependent internal friction (= dissipation).

Combining (56), (57), we deduce for any cyclic process Γ_1 that

$$\begin{array}{rcl} \int_a^b \frac{\mathcal{Q}(T,V,\dot{T},\dot{V})}{T}dt & = & \int_a^b \frac{d}{dt}S(T,V)dt \\ & + & \int_a^b \frac{R_2(T,V,\dot{T},\dot{V})}{T}dt \\ & = & \int_a^b \frac{R_2(T,V,\dot{T},\dot{V})}{T}dt \\ & \leq & 0. \end{array} \tag{57}$$

We employ earlier notation to rewrite:

$$\int_\Gamma \frac{đ\, Q}{T} \leq 0. \qquad \Gamma \text{ a cyclic process} \tag{58}$$

This is a form of *Clausius' inequality*. If Γ is a process from the state $\alpha = (T_0, V_0)$ to $\beta = (T_1, V_1)$, we likewise deduce

$$\int_\Gamma \frac{đ\, Q}{T} \leq S(\beta) - S(\alpha). \tag{59}$$

Lastly, note for our model that if Γ is a cyclic process with maximum temperature T_2 and minimum temperature T_1, its efficiency is

$$\eta \leq 1 - \frac{T_1}{T_2}.$$

The proof is precisely like that in §3, except that we write

$$q(t) = \mathcal{Q}(T(t), V(t), \dot{T}(t), \dot{V}(t))$$

and start with the inequality

$$0 \geq \int_\Gamma \frac{đ\, Q}{T} = \int_a^b \frac{q}{T}dt.$$

□

B. Some general theories

In this section we discuss two representative modern theories for thermodynamics.

1. Entropy and efficiency

First we follow Day–Silhavý [D-S] and introduce a new mathematical model for thermodynamic systems.

a. Definitions

Notation. $(Y_1, \ldots, Y_n) = Y =$ typical point in $\mathbb{R}^n$.

A model for a thermodynamic system in many variables

We are given:

(a) an open, simply connected subset Σ of $\mathbb{R}^n$ (Σ is the *state space* and elements of Σ are called *states*)

and

(b) two C^2 functions

$$\begin{cases} T : \Sigma \to (0, \infty) \\ \Lambda : \Sigma \to \mathbb{R}^n. \end{cases}$$

T is the *temperature* and the components of Λ are the *generalized latent heats*

$$\Lambda = (\Lambda^1, \ldots, \Lambda^n).$$

Notation.

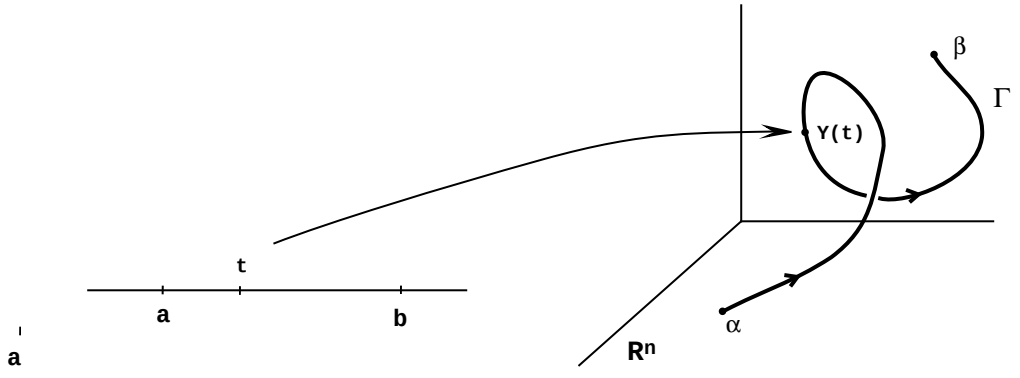
(a) A *path* Γ is an oriented, continuous, piecewise C^1 curve in Σ. A path is a *cycle* if its starting and end points coincide.

(b) If Γ is a path, its *reversal* $\hat{\Gamma}$ is the path taken with opposite orientation.

(c) If Γ_1 and Γ_2 are two paths such that the endpoint of Γ_1 is the starting point of Γ_2, we write

$$\Gamma_2 * \Gamma_1$$

to denote the path consisting of Γ_1, followed by Γ_2.



Note. We parameterize Γ by writing $\{Y(t) \mid a \le t \le b\}$

$$Y(t) = (Y_1(t), \ldots, Y_n(t)) = \textit{ state} \text{ at time } t$$

$\hat{\Gamma}, \Gamma_2 * \Gamma_1$ have the obvious parameterizations. □

Definitions. (i)

$$\begin{aligned} \mathbb{Q}(\Gamma) &= \int_\Gamma đ Q = \int_\Gamma \Lambda \cdot dY = \int_a^b \Lambda(Y(t)) \cdot \dot{Y}(t) dt \\ &= \textit{ heat absorbed} \text{ along } \Gamma. \end{aligned}$$

(ii)

$$\begin{aligned} q(t) &= \Lambda(Y(t)) \cdot \dot{Y}(t) = \textit{ heating at time } t \\ q^+(t) &= \begin{cases} q(t) & \text{if } q(t) \ge 0 \\ 0 & \text{if } q(t) \le 0 \end{cases} \\ q^-(t) &= \begin{cases} 0 & \text{if } q(t) \ge 0 \\ -q(t) & \text{if } q(t) \le 0. \end{cases} \end{aligned}$$

(iii) If Γ is a path,

$$\begin{aligned} \mathbb{Q}^+(\Gamma) &= \int_a^b q^+ dt = \textit{ heat gained along } \Gamma \\ \mathbb{Q}^-(\Gamma) &= \int_a^b q^- dt = \textit{ heat lost along } \Gamma. \end{aligned}$$

If Γ is a cycle,

$$\mathbb{W}(\Gamma) = \mathbb{Q}(\Gamma) = \mathbb{Q}^+(\Gamma) - \mathbb{Q}^-(\Gamma) = \textit{ work performed along } \Gamma.$$

(iv)

$$\begin{aligned} t^+(\Gamma) &= \{t \in [a,b] \mid \dot{Y}(t) \text{ exists}, q(t) > 0\} = \textit{ times at which heat is gained} \\ t^-(\Gamma) &= \{t \in [a,b] \mid \dot{Y}(t) \text{ exists}, q(t) < 0\} = \textit{ times at which heat is emitted.} \end{aligned}$$

(v)

$$\begin{aligned} T^+(\Gamma) &= \sup\{T(Y(t)) \mid t \in t^+(\Gamma) \cup t^-(\Gamma)\} \\ &= \textit{maximum temperature} \text{ at which heat is absorbed or emitted} \\ T^-(\Gamma) &= \min\{T(Y(t)) \mid t \in t^+(\Gamma) \cup t^-(\Gamma)\} \\ &= \textit{minimum temperature} \text{ at which heat is absorbed or emitted.} \end{aligned}$$

Remark.

$$\begin{aligned}
\mathbb{Q}^+(\Gamma) &= \mathbb{Q}^-(\hat{\Gamma}) \\
\mathbb{Q}^-(\Gamma) &= \mathbb{Q}^+(\hat{\Gamma}) \\
\mathbb{Q}(\Gamma) &= -\mathbb{Q}(\hat{\Gamma}) \\
T^+(\Gamma) &= T^+(\hat{\Gamma}) \\
T^-(\Gamma) &= T^-(\hat{\Gamma}).
\end{aligned}$$

□

Terminology: A path Γ is called

		Abbreviations
(a)	*adiabatic* if $t^+(\Gamma), t^-(\Gamma) = \emptyset$.	A
(b)	*absorbing and essentially isothermal* if $t^-(\Gamma) = \emptyset$, $t^+(\Gamma) \neq \emptyset$ and $T(Y(t))$ is constant on $t^+(\Gamma)$.	M^+
(c)	*emitting and essentially isothermal* if $t^+(\Gamma) = \emptyset$, $t^-(\Gamma) \neq \emptyset$ and $T(Y(t))$ is constant on $t^-(\Gamma)$.	M^-
(d)	*monotonic and essentially isothermal* if Γ is one of types (a), (b), (c) above.	M
(e)	*essentially isothermal* if $T(Y(t))$ is constant on $t^+(\Gamma) \cup t^-(\Gamma)$.	I
(f)	*a Carnot path* if there exist $T_1 \leq T_2$ such that	C

$$\begin{aligned}
T(Y(t)) &= T_1 \text{ if } t \in t^-(\Gamma) \\
T(Y(t)) &= T_2 \text{ if } t \in t^+(\Gamma).
\end{aligned}$$

□

Notation. If $\alpha, \beta \in \Sigma$,

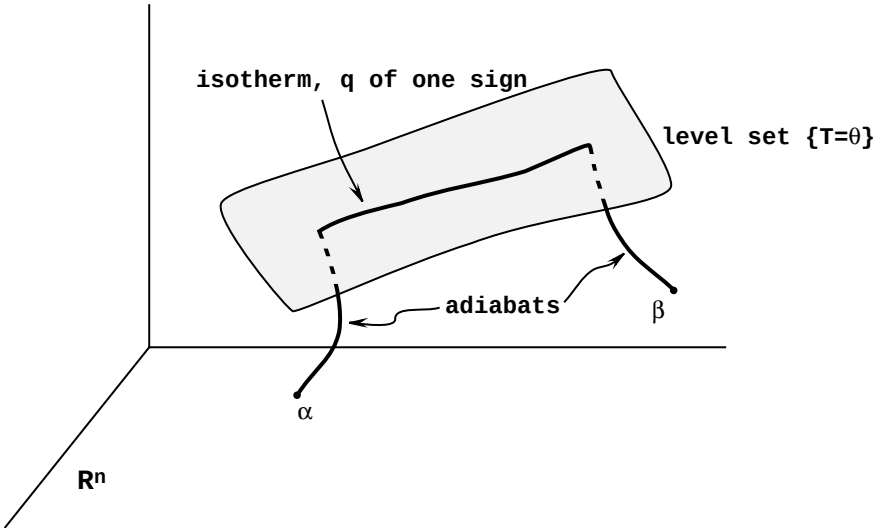
$$\begin{aligned}
P(\alpha, \beta) &= \text{collection of all paths from } \alpha \text{ to } \beta \text{ in } \Sigma \\
A(\alpha, \beta) &= \text{collection of all adiabatic paths from } \alpha \text{ to } \beta.
\end{aligned}$$

$M^{\pm}(\alpha, \beta)$, $M(\alpha, \beta)$, $I(\alpha, \beta)$, $C(\alpha, \beta)$ are similarly defined. □

b. Existence of S

Main Hypothesis. We assume that for each pair of states $\alpha, \beta \in \Sigma$ and for each temperature level θ attained in Σ, there exists a monotone, essentially isothermal path $\Gamma \in M(\alpha, \beta)$ such that

$$T(Y(t)) = \theta \text{ on } t^+(\Gamma) \cup t^-(\Gamma). \tag{1}$$



Theorem. *Assume*

$$\mathbb{W}(\Gamma) \leq \left(1 - \frac{T^-(\Gamma)}{T^+(\Gamma)}\right) \mathbb{Q}^+(\Gamma) \tag{2}$$

for each cycle in Σ *and*

$$\mathbb{W}(\Gamma) = \left(1 - \frac{T^-(\Gamma)}{T^+(\Gamma)}\right) \mathbb{Q}^+(\Gamma) \tag{3}$$

for each Carnot cycle in Σ.

Then there exists a C^2 *function*

$$S : \Sigma \to \mathbb{R}$$

such that

$$\frac{\partial S}{\partial Y_k} = \frac{\Lambda^k}{T} \quad \text{in } \Sigma \ (k = 1, 2, \ldots, n). \tag{4}$$

This result says that the *efficiency estimates* (2), (3) (special cases of which we have earlier encountered) in fact imply the existence of the entropy S. Conversely it is easy to check using the arguments in §A.3 that (4) implies (2), (3).

Proof. 1. Define the *crude entropy change*

$$\xi(\Gamma) := \begin{cases} 0 & \text{if } \Gamma \text{ is adiabatic} \\ \frac{\mathbb{Q}^+(\Gamma)}{T^+(\Gamma)} - \frac{\mathbb{Q}^-(\Gamma)}{T^-(\Gamma)} & \text{if not.} \end{cases} \tag{5}$$

Then (2), (3) say:

$$\text{(6)} \qquad \begin{cases} \xi(\Gamma) \le 0 & \text{for each cycle } \Gamma, \\ \xi(\Gamma) = 0 & \text{for each Carnot cycle } \Gamma. \end{cases}$$

2. **Claim # 1**. For each $\alpha, \beta \in \Sigma$:

$$\text{(7)} \qquad \begin{cases} M(\alpha,\beta) = A(\alpha,\beta) & or \quad M(\alpha,\beta) = M^+(\alpha,\beta) \\ & or \quad M(\alpha,\beta) = M^-(\alpha,\beta). \end{cases}$$

To prove this, fix $\alpha, \beta \in \Sigma$, $\Gamma_1, \Gamma_2 \in M(\alpha,\beta)$. Assume first $\Gamma_1 \in M^+(\alpha,\beta)$, but $\Gamma_2 \notin M^+(\alpha,\beta)$. Then $\Gamma_2 \in A(\alpha,\beta) \cup M^-(\alpha,\beta)$, and so $\mathbb{Q}^+(\Gamma_2) = \mathbb{Q}^-(\Gamma_1) = 0$. Hence $\mathbb{Q}^-(\hat{\Gamma}_2 * \Gamma_1) = \mathbb{Q}^-(\hat{\Gamma}_2) + \mathbb{Q}^-(\Gamma_1) = \mathbb{Q}^+(\Gamma_2) + \mathbb{Q}^-(\Gamma_1) = 0$, but $\hat{\Gamma}_2 * \Gamma_1$ is *not* adiabatic. Thus

$$\begin{aligned} \xi(\hat{\Gamma}_2 * \Gamma_1) &= \tfrac{\mathbb{Q}^+(\hat{\Gamma}_2 * \Gamma_1)}{T^+(\hat{\Gamma}_2 * \Gamma_1)} \\ &= \tfrac{\mathbb{Q}^+(\hat{\Gamma}_2) + \mathbb{Q}^+(\Gamma_1)}{T^+(\hat{\Gamma}_2 * \Gamma_1)} \\ &= \tfrac{\mathbb{Q}^-(\Gamma_2) + \mathbb{Q}^+(\Gamma_1)}{T^+(\hat{\Gamma}_2 * \Gamma_1)} > 0. \end{aligned}$$

Since $\hat{\Gamma}_2 * \Gamma_1$ is a cycle, we have a contradiction to (6). Hence $\Gamma_1 \in M^+(\alpha,\beta)$ implies $\Gamma_2 \in M^+(\alpha,\beta)$. Likewise $\Gamma_1 \in M^-(\alpha,\beta)$ implies $\Gamma_2 \in M^-(\alpha,\beta)$. This proves (7).

3. **Claim # 2**. If $\Gamma_1, \Gamma_2 \in M(\alpha,\beta)$, then

$$\text{(8)} \qquad \xi(\Gamma_1) = \xi(\Gamma_2).$$

According to Claim # 1, $\Gamma_1, \Gamma_2 \in A(\alpha,\beta)$ *or* $\Gamma_1, \Gamma_2 \in M^+(\alpha,\beta)$ *or* $\Gamma_1, \Gamma_2 \in M^-(\alpha,\beta)$.

The first possibility immediately gives (8). Suppose now $\Gamma_1, \Gamma_2 \in M^+(\alpha,\beta)$, with $\mathbb{Q}^+(\Gamma_1) \ge \mathbb{Q}^+(\Gamma_2)$. Then $\Gamma = \hat{\Gamma}_2 * \Gamma_1$ is cyclic, with

$$\begin{cases} T^+(\Gamma) = T^+(\Gamma_1) \\ T^-(\Gamma) = T^+(\Gamma_2) \\ \mathbb{Q}^+(\Gamma) = \mathbb{Q}^+(\Gamma_1) \\ \mathbb{Q}^-(\Gamma) = \mathbb{Q}^+(\Gamma_2). \end{cases}$$

Thus (6) implies

$$\begin{aligned} 0 = \xi(\Gamma) &= \tfrac{\mathbb{Q}^+(\Gamma)}{T^+(\Gamma)} - \tfrac{\mathbb{Q}^-(\Gamma)}{T^-(\Gamma)} \\ &= \tfrac{Q^+(\Gamma_1)}{T^+(\Gamma_1)} - \tfrac{Q^+(\Gamma_2)}{T^+(\Gamma_2)} \\ &= \xi(\Gamma_1) - \xi(\Gamma_2). \end{aligned}$$

This is (8) and a similar proof is valid if $\Gamma_1, \Gamma_2 \in M^-(\alpha,\beta)$.

4. **Claim # 3**. If $\Delta \in P(\alpha,\beta)$ and $\Gamma \in M(\alpha,\beta)$, then

$$\xi(\Delta) \leq \xi(\Gamma) \tag{9}$$

To prove (9), recall the possibilities listed in (7). If $M(\alpha,\beta) = A(\alpha,\beta)$, then Γ is adiabatic and $\xi(\Gamma) = 0$. Also $\hat{\Gamma} * \Delta$ is a cycle, and $\xi(\hat{\Gamma} * \Delta) = \xi(\Delta)$. Thus (6) implies

$$\xi(\Delta) = \xi(\hat{\Gamma} * \Delta) \leq 0 = \xi(\Gamma).$$

This is (9).

If $M(\alpha,\beta) = M^+(\alpha,\beta)$, then $A(\alpha,\beta) = M^-(\alpha,\beta) = \emptyset$ and so Δ is not adiabatic. Thus $T^-(\Delta)$ is defined. According to the Main Hypothesis, there exists $\Pi \in M(\alpha,\beta) = M^+(\alpha,\beta)$ such that

$$T^+(\Pi) = T^-(\Delta).$$

Set $\Xi = \hat{\Pi} * \Delta$. Then Ξ is a cycle, with

$$\begin{cases} T^+(\Xi) = T^+(\Delta) \\ T^-(\Xi) = T^+(\Pi) = T^-(\Delta) \\ \mathbb{Q}^+(\Xi) = \mathbb{Q}^+(\Delta) \\ \mathbb{Q}^-(\Xi) = \mathbb{Q}^-(\Delta) + \mathbb{Q}^+(\Pi) \end{cases}$$

Thus (6) says

$$\begin{aligned} 0 &\geq \xi(\Xi) \\ &= \tfrac{\mathbb{Q}^+(\Xi)}{T^+(\Xi)} - \tfrac{Q^-(\Xi)}{T^-(\Xi)} \\ &= \tfrac{Q^+(\Delta)}{T^+(\Delta)} - \tfrac{Q^-(\Delta)}{T^-(\Delta)} - \tfrac{Q^+(\Pi)}{T^+(\Pi)} \\ &= \xi(\Delta) - \xi(\Pi). \end{aligned}$$

Then

$$\xi(\Delta) \leq \xi(\Pi) = \xi(\Gamma),$$

where we employed Claim # 3 for the last equality. The proof of (9) if $M(\alpha,\beta) = M^-(\alpha,\beta)$ is similar.

5. **Claim # 4**. If $\Delta \in P(\alpha,\beta)$ and $\Gamma \in I(\alpha,\beta)$, then

$$\xi(\Delta) \leq \xi(\Gamma). \tag{10}$$

To verify (10), select any $\Pi \in M(\alpha,\beta)$. Then $\hat{\Pi} \in M(\beta,\alpha)$, $\hat{\Gamma} \in P(\beta,\alpha)$, and so

$$\xi(\hat{\Gamma}) \leq \xi(\hat{\Pi})$$

according to Claim # 3. Since $\Pi, \Gamma \in I(\alpha,\beta)$,

$$\xi(\hat{\Gamma}) = -\xi(\Gamma),\ \xi(\hat{\Pi}) = -\xi(\Pi).$$

Thus

$$\xi(\Pi) \leq \xi(\Gamma).$$

Owing to Claim # 3, then,

$$\xi(\Delta) \leq \xi(\Pi) \leq \xi(\Gamma).$$

This is (10).

6. **Claim # 5**. There is a function $\phi : \Sigma \to \mathbb{R}$ such that

$$\xi(\Gamma) \leq \phi(\beta) - \phi(\alpha) \tag{11}$$

for all $\alpha, \beta \in \Sigma$, $\Gamma \in P(\alpha, \beta)$.

To prove this, note first that Claim # 4 implies

$$\xi(\Delta_1) = \xi(\Delta_2) \text{ if } \Delta_1, \Delta_2 \in I(\alpha, \beta).$$

Thus we can define

$$\pi(\alpha, \beta) := \xi(\Delta) \qquad (\Delta \in I(\alpha, \beta)).$$

Then according to Claim # 4

$$\xi(\Gamma) \leq \pi(\alpha, \beta) \qquad (\Gamma \in P(\alpha, \beta)),$$

and so to derive (11) we must show that we can write

$$\pi(\alpha, \beta) = \phi(\beta) - \phi(\alpha) \qquad \text{for all } \alpha, \beta \in \Sigma. \tag{12}$$

For this fix a state $\gamma \in \Sigma$ and a temperature level θ. Owing to the Main Hypothesis, there exist $\Gamma_1 \in M(\alpha, \beta)$, $\Gamma_2 \in M(\beta, \gamma)$ such that

$$\begin{cases} T^{\pm}(\Gamma_1) = \theta & \text{on } t^+(\Gamma_1) \cup t^-(\Gamma_1) \\ T^{\pm}(\Gamma_2) = \theta & \text{on } t^+(\Gamma_2) \cup t^-(\Gamma_2). \end{cases}$$

Then $\Gamma_2 * \Gamma_1 \in I(\alpha, \gamma)$ and

$$\begin{aligned} \xi(\Gamma_2 * \Gamma_1) &= \tfrac{\mathbb{Q}^+(\Gamma_2 * \Gamma_1)}{T^+(\Gamma_2 * \Gamma_1)} - \tfrac{\mathbb{Q}^+(\Gamma_2 * \Gamma_1)}{T^-(\Gamma_2 * \Gamma_1)} \\ &= \tfrac{\mathbb{Q}^+(\Gamma_2) + \mathbb{Q}^+(\Gamma_1)}{\theta} - \tfrac{\mathbb{Q}^-(\Gamma_2) + \mathbb{Q}^-(\Gamma_1)}{\theta} \\ &= \xi(\Gamma_2) + \xi(\Gamma_1). \end{aligned}$$

Hence

$$\pi(\alpha, \gamma) = \pi(\alpha, \beta) + \pi(\beta, \gamma). \tag{13}$$

Define

$$\phi(\alpha) := -\pi(\alpha, \gamma),$$

to deduce (12) from (13).

7. Finally we build the entropy function S. Take any cycle Γ in Σ, Γ parameterized by

$$\{Y(t) \mid 0 \le t \le 1\}.$$

Fix $\varepsilon > 0$. Then take N so large that

$$\left| \frac{1}{T(Y(t_1))} - \frac{1}{T(Y(t_2))} \right| \le \varepsilon$$

if $t_1, t_2 \in \left[\frac{k-1}{N}, \frac{k}{N}\right]$ $(k = 1, \ldots, N)$. Thus we have

$$0 \le \frac{1}{T^-(\Gamma_k)} - \frac{1}{T^+(\Gamma_k)} \le \varepsilon \qquad (k = 1, \ldots, N), \tag{14}$$

where Γ_k is parameterized by $\left\{Y(t) \mid \frac{k-1}{N} \le t \le \frac{k}{N}\right\}$. We here and afterwards assume each Γ_k is not adiabatic, as the relevant estimates are trivial for any adiabatic Γ_k. Thus

$$\begin{aligned}
\int_\Gamma \frac{đ Q}{T} &:= \int_0^1 \frac{1}{T(Y(t))} \underbrace{\Lambda(Y(t)) \cdot \dot{Y}(t)}_{q(t)} dt \\
&= \sum_{k=1}^N \int_{\frac{k-1}{N}}^{\frac{k}{N}} \frac{1}{T(Y(t))} q(t) dt \\
&\le \sum_{k=1}^N \frac{Q^+(\Gamma_k)}{T^-(\Gamma_k)} - \frac{\mathbb{Q}^-(\Gamma_k)}{T^+(\Gamma_k)} \\
&\le \sum_{k=1}^N Q^+(\Gamma_k) \left(\frac{1}{T^+(\Gamma_k)} + \varepsilon\right) + \left(-\frac{1}{T^-(\Gamma_k)} + \varepsilon\right) \mathbb{Q}^-(\Gamma_k) \\
&= \sum_{k=1}^N \xi(\Gamma_k) + \varepsilon(\mathbb{Q}^+(\Gamma_k) + \mathbb{Q}^-(\Gamma_k)) \\
&= \sum_{k=1}^N \xi(\Gamma_k) + \varepsilon \int_0^1 |q(t)| dt \\
&\le \sum_{k=1}^N \xi(\Gamma_k) + C\varepsilon.
\end{aligned}$$

Now

$$\xi(\Gamma_k) \le \phi(\beta_k) - \phi(\alpha_k)$$

by Claim # 5, with

$$\begin{aligned}
\alpha_k &= Y\left(\tfrac{k-1}{N}\right) \\
\beta_k &= Y\left(\tfrac{k}{N}\right) = \alpha_{k+1}.
\end{aligned}$$

Since Γ is a cycle, $\alpha_{N+1} = \alpha_1$, and so

$$\sum_{k=1}^n \xi(\Gamma_k) \le 0.$$

Consequently the calculation above forces:

$$\int_0^1 \frac{\Lambda(Y(t))}{T(Y(t))}\dot{Y}(t)dt \leq C\varepsilon,$$

and thus

$$\int_\Gamma \frac{đ Q}{T} = \int_0^1 \frac{q(t)}{T(Y(t))}dt \leq 0.$$

Applying the same reasoning to $\hat{\Gamma}$ in place of Γ, we conclude

$$\int_\Gamma \frac{đ Q}{T} = 0 \text{ for each cycle } \Gamma.$$

As Σ is simply connected, this fact implies the existence of $S : \Sigma \to \mathbb{R}$ with

$$DS = \frac{\Lambda}{T}.$$

□

2. Entropy, temperature and supporting hyperplanes

Modern rigorous approaches to thermodynamics vastly extend the realm of applicability of the foregoing notions to extremely diverse systems of various sorts. See for instance Serrin [S2], [S3]. As an interesting second illustration of a modern theory we next present Feinberg and Lavine's derivation [F-L1] of entropy *and temperature* for an abstract thermal system, as a consequence of the Hahn–Banach Theorem.

a. Definitions

Notation.

(i) Σ = a compact metric space.

(ii) $C(\Sigma)$ = space of continuous functions $\phi : \Sigma \to \mathbb{R}$, with

$$\|\phi\|_{C(\Sigma)} = \max_{\alpha\in\Sigma} |\phi(\alpha)|.$$

(iii) $\mathcal{M}(\Sigma)$ = space of signed Radon measures on Σ.

$\mathcal{M}_+(\Sigma)$ = space of nonnegative Radon measures.

$\mathcal{M}_0(\Sigma) = \{\nu \in \mathcal{M}(\Sigma) \mid \nu(\Sigma) = 0\}$.

(iv) We endow $\mathcal{M}(\Sigma)$ with the *weak* topology*, which is the weakest topology for which the mappings

$$\mu \mapsto \int_\Sigma \phi d\mu$$

are continuous on $\mathcal{M}(\Sigma)$ for all $\phi \in C(\Sigma)$.

(v) $\mathcal{M}_0(\Sigma) \times \mathcal{M}(\Sigma) = \{(\nu, \mu) \mid \nu \in \mathcal{M}_0(\Sigma),\ \mu \in \mathcal{M}(\Sigma)\}$.

We give $\mathcal{M}(\Sigma)$ the weak* topology, $\mathcal{M}_0(\Sigma)$ the inherited subspace topology and $\mathcal{M}_0(\Sigma) \times \mathcal{M}(\Sigma)$ the product topology. □

A model for an abstract thermodynamic system

We are given

(a) a compact metric space Σ, as above. (Σ is the *state space* and elements of Σ are called *states*).

and

(b) a nonempty set $\mathcal{P} \subset \mathcal{M}_0(\Sigma) \times \mathcal{M}(\Sigma)$, such that

(15) $\mathcal{P}$ is a closed, convex cone.

(Elements of $\mathcal{P}$ are called *processes*. If $\Gamma = (\nu, \mu) \in \mathcal{P}$ is a process, then

$$\nu \in \mathcal{M}_0(\Sigma) \text{ is the } \textit{change of condition}$$

and

$$\mu \in \mathcal{M}(\Sigma) \text{ is the } \textit{heating measure}$$

for Γ.)

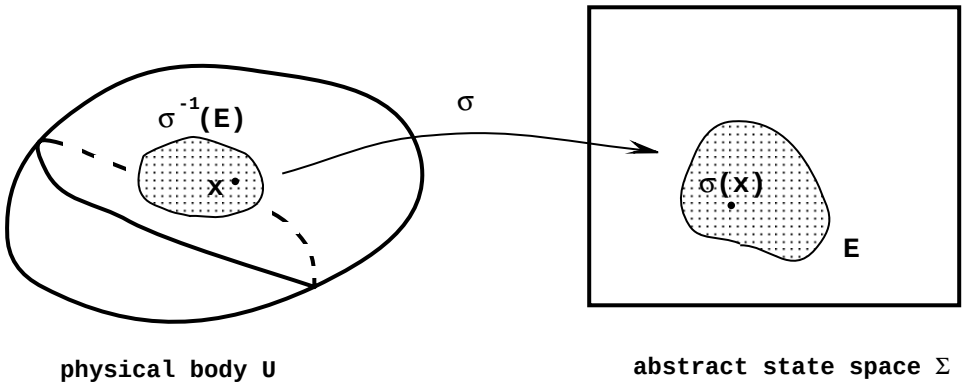
Definitions. (i) A *cyclic process* for our system is a process whose change of condition is the zero measure.

(ii) Let $\mathcal{C}$ denote the set of measures which are heating measures for cyclic processes. That is,

(16) $$\mathcal{C} = \{\mu \in \mathcal{M}(\Sigma) \mid (0, \mu) \in \mathcal{P}\}.$$

Physical interpretation. The abstract apparatus above is meant to model the following situation.

(a) Suppose we have a physical body U made of various material points. At any given moment of time, we assign to each point $x \in U$ a *state* $\sigma(x) \in \Sigma$.



The *condition* of the body at this fixed time is then defined to be the measure $\rho \in \mathcal{M}_+(\Sigma)$ such that

$$\rho(E) = \text{ mass of } \sigma^{-1}(E)$$

for each Borel subset $E \subset \Sigma$.

(b) We now image a *process* which somehow acts on U, thereby changing the *initial condition* ρ_i to a *final condition* ρ_f. The *change of condition* is

$$\nu = \rho_f - \rho_i.$$

Observe

$$\begin{aligned} \nu(\Sigma) &= \rho_f(\Sigma) - \rho_i(\Sigma) \\ &= \text{mass of } U - \text{ mass of } U = 0. \end{aligned}$$

Thus $\nu \in \mathcal{M}_0(\Sigma)$. If the process is cyclic, then $\rho_f = \rho_i$; that is, $\nu = 0$.

(c) We record also the heat received during the process by defining

$$\begin{aligned} \mu(E) = &\text{ net amount of heat received from the} \\ &\text{exterior during the entire process, by the} \\ &\text{material points with initial states lying in } E \end{aligned}$$

for each Borel subset $E \subset \Sigma$. The signed measure μ is the *heating measure*. □

b. Second Law

We next assume that our abstract system satisfies a form of the *Second Law*, which for us means

$$\mathcal{C} \cap \mathcal{M}_+(\Sigma) = \{0\}. \tag{17}$$

Physical interpretation. Condition (17) is a mathematical interpretation of the *Kelvin–Planck* statement of the Second Law, namely

$$\text{(18)} \qquad \begin{cases} \text{“if, while suffering a cyclic process, a body absorbs} \\ \text{heat from its exterior, that body must also emit heat} \\ \text{to its exterior during the process”.} \end{cases}$$

This is quoted from [F-L1, p. 223]. In other words, the heat supplied to the body undergoing the cyclic process cannot be converted entirely into work: there must be emission of heat from the body as well. The cyclic process cannot operate with perfect efficiency.

Our condition (17) is a mathematical interpretation of all this: the heating measure μ for a cyclic process cannot be a nonnegative measure.

c. The Hahn–Banach Theorem

We will need a form of the

Hahn–Banach Theorem. *Let X be a Hausdorff, locally convex topological vector space. Suppose K_1, K_2 are two nonempty, disjoint, closed convex subsets of X and that K_1 is a cone.*

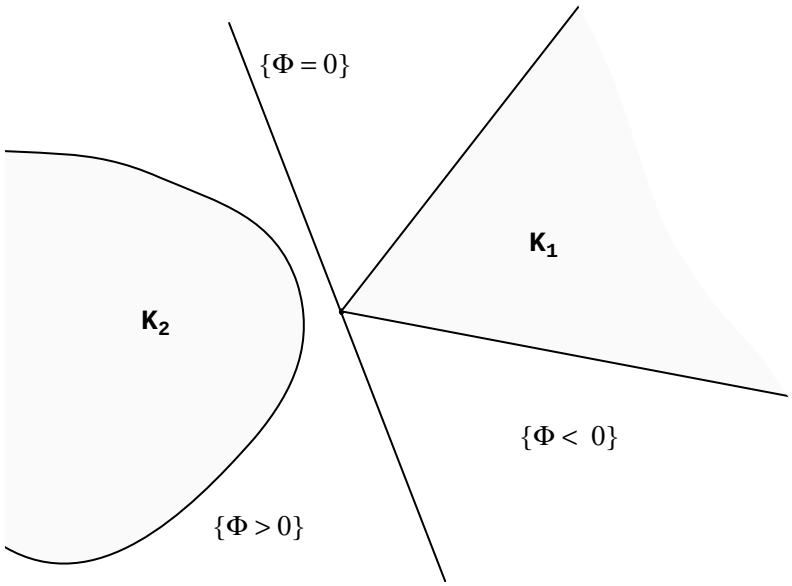
Then there exists a continuous linear function

$$\text{(19)} \qquad \Phi : X \to \mathbb{R}$$

such that

$$\text{(20)} \qquad \begin{cases} \Phi(k_1) \leq 0 \quad \textit{for all } k_1 \in K_1 \\ \Phi(k_2) > 0 \quad \textit{for all } k_2 \in K_2. \end{cases}$$

We can think of the set $\{\Phi = \gamma\}$ as a *separating hyperplane* between K_1, K_2.



To utilize the Hahn–Banach Theorem, we will need an explicit characterization of Φ in certain circumstances:

Lemma (i) *Let $X = \mathcal{M}(\Sigma)$ and suppose*

$$\Phi : X \to \mathbb{R} \tag{21}$$

is continuous and linear. Then there exists $\phi \in C(\Sigma)$ such that

$$\Phi(\mu) = \int_\Sigma \phi d\mu \quad \text{for all } \mu \in X. \tag{22}$$

(ii) *Let $X = \mathcal{M}_0(\Sigma) \times \mathcal{M}(\Sigma)$ and suppose*

$$\Phi : X \to \mathbb{R}$$

is continuous and linear. Then there exist $\phi, \psi \in C(\Sigma)$ such that

$$\Phi((\nu, \mu)) = \int_\Sigma \psi d\nu + \int_\Sigma \phi d\mu \tag{23}$$

for all $(\nu, \mu) \in X$.

Proof. 1. Suppose $X = \mathcal{M}(\Sigma)$ and

$$\Phi : X \to \mathbb{R}$$

is continuous, linear. Fix any point $\alpha \in \Sigma$ and let δ_α denote the point mass at α. Next define

$$\phi(\alpha) := \Phi(\delta_\alpha) \qquad (\alpha \in \Sigma).$$

2. We first claim

$$\phi \in C(\Sigma).$$

To prove this, let $\alpha_k \to \alpha$ in Σ. Then for every $\psi \in C(\Sigma)$,

$$\int_\Sigma \psi d\delta_{\alpha_k} = \psi(\alpha_k) \to \psi(\alpha) = \int_\Sigma \psi d\delta_\alpha$$

and so

$$\delta_{\alpha_k} \to \delta_\alpha \text{ weakly as measures.}$$

This means

$$\delta_{\alpha_k} \to \delta_\alpha \text{ in } \mathcal{M}(\Sigma).$$

As Φ is continuous,

$$\phi(\alpha_k) = \Phi(\delta_{\alpha_k}) \to \Phi(\delta_\alpha) = \phi(\alpha).$$

Thus ϕ is continuous.

3. Since Φ is linear,

$$\Phi\left(\sum_{k=1}^m a_k \delta_{\alpha_k}\right) = \sum_{k=1}^m a_k \phi(\alpha_k) \tag{24}$$

for all $\{\alpha_k\}_{k=1}^m \subset \Sigma$, $\{a_k\}_{k=1}^m \in \mathbb{R}$. Finally take any measure $\mu \in \mathcal{M}(\Sigma)$. We can find measures $\{\mu_m\}_{m=1}^\infty$ of the form

$$\mu_m = \sum_{k=1}^m a_k^m \delta_{\alpha_k^m} \qquad (m = 1, \dots)$$

such that

$$\mu_m \to \mu \text{ in } \mathcal{M}(\Sigma). \tag{25}$$

Then (24) implies

$$\sum_{k=1}^m a_k^m \phi(\alpha_k^m) = \Phi(\mu_m) \to \Phi(\mu) \text{ as } m \to \infty.$$

But since ϕ is continuous, (25) says

$$\int_\Sigma \phi d\mu_m = \sum_{k=1}^m a_k^m \phi(\alpha_k^m) \to \int_\Sigma \phi d\mu \text{ as } m \to \infty.$$

Thus

$$\Phi(\mu) = \int_\Sigma \phi d\mu.$$

This proves the representation formula (22) and the proof of (23) is then immediate. □

d. Existence of S, T

Theorem *Assume that our abstract thermodynamic system satisfies* (17). *Then there exist continuous functions*

$$S : \Sigma \to \mathbb{R}$$
$$T : \Sigma \to (0, \infty)$$

such that

$$\int_\Sigma \frac{d\mu}{T} \leq \int_\Sigma S d\nu \tag{26}$$

for each process $\Gamma = (\nu, \mu) \in \mathcal{P}$.

We will later interpret (26) as a form of Clausius' inequality.

Proof. 1. Hereafter set $X = \mathcal{M}_0(\Sigma) \times \mathcal{M}(\Sigma)$,

$$\begin{cases} K_1 = \mathcal{P} \\ K_2 = \{0\} \times \mathcal{M}_+^1(\Sigma), \end{cases}$$

where

$$\mathcal{M}_+^1(\Sigma) = \{\rho \in \mathcal{M}_+(\Sigma) \mid \rho(\Sigma) = 1\}.$$

By hypothesis (15), K_1 is a closed, convex cone in X. K_2 is also closed, convex in X. In addition our form of the Second Law (17) implies that

$$K_1 \cap K_2 = \emptyset.$$

We may therefore involve the Hahn–Banach Theorem, in the formulation (20), (23): there exist $\phi, \psi \in C(\Sigma)$ with

$$\Phi(\nu, \mu) = \int_\Sigma \psi d\nu + \int_\Sigma \phi d\mu \leq 0 \text{ for all } \Gamma = (\nu, \mu) \in \mathcal{P} \tag{27}$$

and

$$\Phi(0, \rho) = \int_\Sigma \phi d\rho > 0 \text{ for all } \rho \in \mathcal{M}_+^1(\Sigma). \tag{28}$$

Taking $\rho = \delta_\alpha$ in (28), where $\alpha \in \Sigma$, we deduce that

$$\phi > 0 \text{ on } \Sigma.$$

Change notation by writing

$$S := -\psi,\ T := \frac{1}{\phi}.$$

Then (27) reads

$$\int_\Sigma \frac{d\mu}{T} \leq \int_\Sigma S d\nu$$

for all processes $\Gamma = (\nu, \mu) \in \mathcal{P}$. □

Physical interpretation. We can repackage inequality (26) into more familiar form by first of all defining

$$\int_\Gamma \frac{đ Q}{T} := \int_\Sigma \frac{d\mu}{T} \tag{29}$$

for each process $\Gamma = (\nu, \mu)$. Then (26) says

$$\int_\Gamma \frac{đ Q}{T} \leq 0 \qquad \Gamma \text{ a cyclic process.} \tag{30}$$

Fix now any two states $\alpha, \beta \in \Sigma$. Then *if* there exists a process $\Gamma = (\delta_\beta - \delta_\alpha, \mu) \in \mathcal{P}$, (26) and (29) read

$$\int_\Gamma \frac{đ Q}{T} \leq S(\beta) - S(\alpha) \qquad \Gamma \text{ a process from } \alpha \text{ to } \beta. \tag{31}$$

Clearly (30) is a kind of Clausius inequality for our abstract thermodynamic system.

Finally let us say a process $\Gamma = (\delta_\beta - \delta_\alpha, \mu) \in \mathcal{P}$ is *reversible* if $\hat{\Gamma} := (\delta_\alpha - \delta_\beta, -\mu) \in \mathcal{P}$. Then

$$\int_\Gamma \frac{đ Q}{T} = S(\beta) - S(\alpha) \qquad \Gamma \text{ a reversible process from } \alpha \text{ to } \beta.$$

Remark. See Serrin [S2], [S3], Coleman–Owen–Serrin [C-O-S], Owen [O] for another general approach based upon a different, precise mathematical interpretation of the Second Law. Note also the very interesting forthcoming book by Man and Serrin [M-S]. □

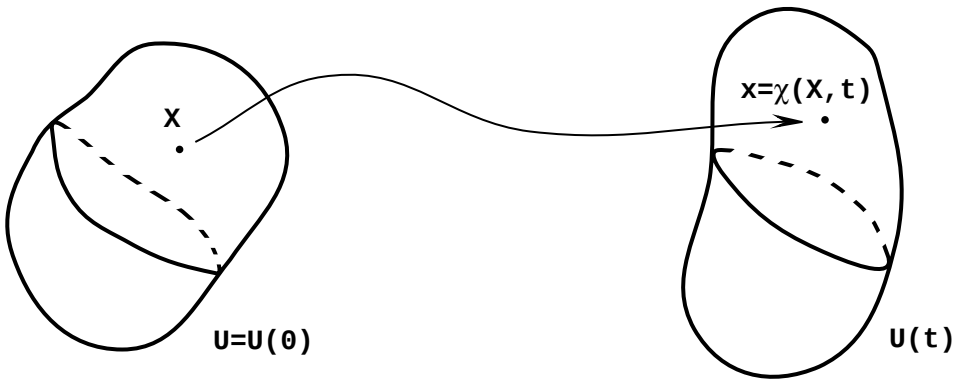
CHAPTER 3: Continuum thermodynamics

Since our primary subject in these notes is the application of entropy ideas to PDE theory, we must next confront a basic issue: the classical physical theory from Chapter I and from §A, B.1 in Chapter II are concerned with entropy defined as an extensive parameter over an entire system. That is, S does not have spatial dependence. The rather abstract framework in §B.2 of Chapter II does on the other hand allow for variations of S over a material body, and this prospect points the way to other modern approaches to *continuum thermodynamics*, for which the entropy, internal energy, temperature, etc. are taken to be functions of both position and time. We will present here the axiomatic method of Coleman–Noll [C-N].

A. Kinematics

1. Deformations

We model the motion of a material body by introducing first a smooth bounded region U, the *reference configuration*, a typical point of which we denote by X. We suppose the moving body occupies the region $U(t)$ at time $t \geq 0$, where for simplicity we take $U(0) = U$.



Let us describe the motion by introducing a smooth mapping $\boldsymbol{\chi} : U \times [0, \infty) \to \mathbb{R}^3$ so that

$$x = \boldsymbol{\chi}(X, T) \tag{1}$$

is the location at time $t \geq 0$ of the material particle initially at $X \in U$. We require that for each $t \geq 0$, $\boldsymbol{\chi}(\cdot, t) : U \to U(t)$ is an orientation preserving diffeomorphism. Write $\boldsymbol{\psi}(\cdot, t) = \boldsymbol{\chi}^{-1}(\cdot, t)$; so that

$$X = \boldsymbol{\psi}(x, t). \tag{2}$$

Then

$$\mathbf{v}(x,t) = \frac{\partial \boldsymbol{\chi}}{\partial t}(X,t) \tag{3}$$

is the *velocity* field, where X, x are associated by (1), (2).

2. Physical quantities

We introduce as well:

(i) the *mass density*

$$\rho(x,t)$$

(ii) the *stress tensor*

$$\mathbf{T}(x,t)$$

(iii) the *body force*/unit mass

$$\mathbf{b}(x,t)$$

(iv) the *internal energy*/unit mass

$$e(x,t)$$

(v) the *heat flux* vector

$$\mathbf{q}(x,t)$$

(vi) the *heat supply*/unit mass

$$r(x,t)$$

(vii) the *entropy*/unit mass

$$s(x,t)$$

(viii) the *local temperature*

$$\theta(x,t).$$

The functions ρ, θ are assumed to be positive.

Remarks. (1) We henceforth assume these are all smooth functions. Note

$$\begin{cases} \rho, e, r, s \text{ and } \theta \text{ are real valued} \\ \mathbf{b}, \mathbf{q} \text{ take values in } \mathbb{R}^3 \\ \mathbf{T} \text{ takes values in } \mathbb{S}^3 \ (= \text{space of } 3 \times 3 \text{ symmetric matrices}) \end{cases}$$

(2) We will sometimes think of these quantities as being functions of the material point X rather than the position x. In this case we will write

$$\rho = \rho(X,t), \ \mathbf{T} = \mathbf{T}(X,t), \ \text{etc.}$$

where X, x are related by (1), (2). □

Notation. We will often write

$$dm = \rho dx. \tag{4}$$

Note. The *kinetic energy* at time $t \geq 0$ is

$$K(t) = \int_{U(t)} \frac{|\mathbf{v}|^2}{2} dm;$$

the *internal energy* is

$$E(t) = \int_{U(t)} e dm;$$

and the *entropy* is

$$S(t) = \int_{U(t)} s dm.$$

□

3. Kinematic formulas

Take V to be any smooth subregion of U and write $V(t) = \boldsymbol{\chi}(V, t)$, $(t \geq 0)$.

If $f = f(x, t)$ $(x \in \mathbb{R}^3,\ t \geq 0)$ is smooth, we compute:

$$\frac{d}{dt}\left(\int_{V(t)} f dx\right) = \int_{V(t)} \frac{\partial f}{\partial t} dx + \int_{\partial V(t)} f \mathbf{v} \cdot \boldsymbol{\nu} dS,$$

where "dS" denotes 2-dimensional surface measure on $\partial V(t)$, $\mathbf{v}$ is the velocity field and $\boldsymbol{\nu}$ is the unit outer normal vector field to $\partial V(t)$. Applying the Gauss–Green Theorem we deduce:

$$\frac{d}{dt}\left(\int_{V(t)} f dx\right) = \int_{V(t)} \frac{\partial f}{\partial t} + \text{ div}(f\mathbf{v}) dx. \tag{5}$$

Take $f = \rho$ above. Then

$$\int_{V(t)} \frac{\partial \rho}{\partial t} + \text{ div}(\rho \mathbf{v}) dx = \frac{d}{dt}\left(\int_{V(t)} \rho dx\right) = 0,$$

as the total mass within the regions $V(t)$ moving with the deformation is unchanging in time. Since the region $V(t)$ is arbitrary, we deduce

$$\frac{\partial \rho}{\partial t} + \text{ div}(\rho \mathbf{v}) = 0 \qquad \textit{conservation of mass.} \tag{6}$$

This PDE holds in $U(t)$ at each time $t \geq 0$. Now again take $f = f(x,t)$ and compute

$$\begin{aligned} \frac{d}{dt}\left(\int_{V(t)} f dm\right) &= \frac{d}{dt}\left(\int_{V(t)} f\rho dx\right) \text{ by (4)} \\ &= \int_{V(t)} \frac{\partial(f\rho)}{\partial t} + \text{ div}(f\rho\mathbf{v})dx \text{ by (5)} \\ &= \int_{V(t)} \frac{\rho\partial f}{\partial t} + \rho\mathbf{v}\cdot Df dx \text{ by (6)}, \end{aligned}$$

where

$$Df = D_x f = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \frac{\partial f}{\partial x_3}\right) = \begin{array}{l}\text{gradient of } f \text{ with} \\ \text{respect to the spatial} \\ \text{variables } x = (x_1, x_2, x_3).\end{array}$$

Recalling (4) we deduce

$$\frac{d}{dt}\left(\int_{V(t)} f dm\right) = \int_{V(t)} \frac{Df}{Dt} dm, \tag{7}$$

where

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + \mathbf{v}\cdot Df$$

is the *material derivative*. Observe that

$$\frac{d}{dt} f(\boldsymbol{\chi}(X,t),t) = \frac{Df}{Dt}.$$

4. Deformation gradient

We define as well the *deformation gradient*

$$\begin{aligned} F(X,t) &= D_X\boldsymbol{\chi}(X,T) \\ &= \begin{pmatrix} \frac{\partial\chi^1}{\partial X_1} & \cdots & \frac{\partial\chi^1}{\partial X_3} \\ & \ddots & \\ \frac{\partial\chi^3}{\partial X_1} & & \frac{\partial\chi^3}{\partial X_3} \end{pmatrix} \end{aligned} \tag{8}$$

and the *velocity gradient*

$$L(X,t) = \frac{\partial F}{\partial t}(X,t)F^{-1}(X,t) \tag{9}$$

for $X \in U$, $t \geq 0$.

To understand the name of L, recall $\mathbf{v}(x,t) = \frac{\partial \boldsymbol{\chi}}{\partial t}(X,t) = \frac{\partial \boldsymbol{\chi}}{\partial t}(\boldsymbol{\psi}(x,t),t)$. Thus

$$v^i_{x_j} = \sum_{k=1}^{3} \frac{\partial^2 \chi^i}{\partial t \partial X_k} \frac{\partial \psi^k}{\partial x_j} \qquad (1 \le i,j \le 3).$$

As $F^{-1} = D_x \boldsymbol{\psi}$, we see that

$$D\mathbf{v}(x,t) = \frac{\partial F}{\partial t}(X,t) F^{-1}(X,t).$$

Thus

$$L(X,t) = D\mathbf{v}(x,t) \tag{10}$$

is indeed the velocity of the gradient.

Remark. Let $\rho(\cdot,0) = \rho_0$ denote the mass density at time $t = 0$. Then

$$\rho(x,t) = (\det\ D_x \boldsymbol{\psi}(x,t))\rho_0(X)$$

is the density at $x \in U(t)$, $t \ge 0$. Since $F = (D_x \boldsymbol{\psi})^{-1}$, we see that

$$\rho(x,t) = (\det\ F(X,t))^{-1} \rho_0(X) \tag{11}$$

for $t \ge 0$, X, x associated by (1), (2).

B. Conservation laws; Clausius–Duhem inequality

We now further assume for each moving subregion $V(t)$ $(t \ge 0)$ as above that we have:

I. Balance of linear momentum

$$\frac{d}{dt}\left(\int_{V(t)} \mathbf{v} dm\right) = \int_{V(t)} \mathbf{b} dm + \int_{\partial V(t)} \mathbf{T}\boldsymbol{\nu} dS. \tag{1}$$

This says the rate of change of linear momentum within the moving region $V(t)$ equals the body force acting on $V(t)$ plus the contact force acting on $\partial V(t)$. We employ (6), (7) in §A and the Gauss–Green Theorem to deduce from (1) that

$$\rho \frac{D\mathbf{v}}{Dt} = \rho \mathbf{b} + \text{ div } \mathbf{T} \qquad \textit{balance of momentum.} \tag{2}$$

We additionally suppose:

II. Energy balance

$$\begin{aligned} \frac{d}{dt}\left(\int_{V(t)} \frac{|v|^2}{2} + e dm\right) &= \int_{V(t)} \mathbf{v}\cdot\mathbf{b} + r dm \\ &+ \int_{\partial V(t)} \mathbf{v}\cdot\mathbf{T}\boldsymbol{\nu} - \mathbf{q}\cdot\boldsymbol{\nu} dS \end{aligned} \tag{3}$$

This identity asserts that the rate of change of the total energy (= kinetic energy + internal energy (including potential energy)) within the moving region $V(t)$ equals the rate of work performed by the body and contact forces, plus the body heat supplied minus the heat flux outward through $\partial V(t)$.

Since $\mathbf{T}$ is symmetric, $\mathbf{v}\cdot\mathbf{T}\boldsymbol{\nu} = (\mathbf{T}\mathbf{v})\cdot\boldsymbol{\nu}$. Hence (3) and the Gauss–Green Theorem imply:

$$\rho\frac{D}{Dt}\left(\frac{|v|^2}{2} + e\right) = \rho(\mathbf{v}\cdot\mathbf{b} + r) + \text{ div}(\mathbf{T}\mathbf{v} - \mathbf{q}).$$

Simplify, using (2) to deduce:

$$\rho\frac{De}{Dt} = \rho r - \text{ div } \mathbf{q} + \mathbf{T} : D\mathbf{v} \qquad \textit{energy balance.} \tag{4}$$

Notation. If A, B are 3×3 matrices, we write

$$A : B = \sum_{i,j=1}^{3} a_{ij}b_{ij}.$$

□

Lastly we hypothesize the

III. Clausius–Duhem inequality

$$\frac{d}{dt}\left(\int_{V(t)} s dm\right) \geq \int_{V(t)} \frac{r}{\theta} dm - \int_{\partial V(t)} \frac{\mathbf{q}\cdot\boldsymbol{\nu}}{\theta} dS. \tag{5}$$

This asserts that the rate of entropy increase within the moving region $V(t)$ is *greater than or equal to* the heat supply divided by temperature integrated over the body plus an *entropy flux* term integrated over $\partial V(t)$. Observe that (5) is a kind of continuum version of the various forms of Clausius' inequality we have earlier encountered.

As before (5) implies

$$\rho\frac{Ds}{Dt} \geq \frac{r\rho}{\theta} - \text{ div}\left(\frac{\mathbf{q}}{\theta}\right) \qquad \textit{entropy inequality.} \tag{6}$$

Notation. We define the *local production of entropy* per unit mass to be:

$$\begin{cases} \gamma &= \dfrac{Ds}{Dt} - \dfrac{r}{\theta} + \dfrac{1}{\rho}\,\text{div}\left(\dfrac{\mathbf{q}}{\theta}\right) \\ &= \dfrac{Ds}{Dt} - \dfrac{r}{\theta} + \dfrac{\text{div}(\mathbf{q})}{\rho\theta} - \dfrac{\mathbf{q}\cdot D\theta}{\rho\theta^2} \\ &\geq 0. \end{cases} \tag{7}$$

□

We call a motion $\boldsymbol{\chi}$ and a collection of functions $\rho, \mathbf{T}, \mathbf{b}$, etc. satisfying I–III above an *admissible thermodynamic process.*

C. Constitutive relations

A particular material is defined by adding to the foregoing additional *constitutive relations*, which are restrictions on the functions $\mathbf{T}, \mathbf{b}$, etc. describing the thermodynamic process.

1. Fluids

Notation. We refer to

$$v = \frac{1}{\rho} \tag{1}$$

as the *specific volume*. Note that then

$$|U(t)| = \int_{U(t)} v dm = \text{ volume of } U(t).$$

□

a. We call our body a *perfect fluid with heat conduction* if there exist four functions $\hat{e}, \hat{\theta}, \hat{T}, \hat{\mathbf{q}}$ such that

$$\begin{cases} \text{(a)} & e = \hat{e}(s, v) \\ \text{(b)} & \theta = \hat{\theta}(s, v) \\ \text{(c)} & \mathbf{T} = \hat{\mathbf{T}}(s, v) \\ \text{(d)} & \mathbf{q} = \hat{\mathbf{q}}(s, v, D\theta). \end{cases} \tag{2}$$

These are the *constitutive relations*.

Notation. Formula (a) means

$$e(x,t) = \hat{e}(s(x,t), v(x,t)) \qquad (x \in U(t),\ t \geq 0)$$

where

$$\hat{e} : \mathbb{R} \times \mathbb{R} \to \mathbb{R}.$$

Equations (b)–(d) have similar interpretations. Below we will sometimes omit writing the $\hat{}$ and so regard e as a function of (s, v), etc. □

The key question is this:

> *What restrictions on the constitutive relations*
> (2) *are imposed by the Clausius–Duhem*
> *inequality?*

To deduce useful information, let us first combine (4), (6) from §B:

$$0 \leq \rho\theta\gamma = \rho\left(\theta\frac{Ds}{Dt} - \frac{De}{Dt}\right) + \mathbf{T} : D\mathbf{v} - \frac{1}{\theta}\mathbf{q} \cdot D\theta. \tag{3}$$

Owing to (2)(a) we have:

$$\frac{De}{Dt} = \frac{\partial\hat{e}}{\partial s}\frac{Ds}{Dt} + \frac{\partial\hat{e}}{\partial v}\frac{Dv}{Dt}. \tag{4}$$

Now the conservation of mass (6) in §A implies

$$\frac{D\rho}{Dt} = -\rho \text{ div } \mathbf{v}.$$

Thus

$$\frac{Dv}{Dt} = -\frac{1}{\rho^2}\frac{D\rho}{Dt} = \frac{1}{\rho} \text{ div } \mathbf{v} = v \text{ div } \mathbf{v}. \tag{5}$$

Insert (4), (5) into (3):

$$0 \leq \rho\left(\hat{\theta} - \frac{\partial\hat{e}}{\partial s}\right)\frac{Ds}{Dt} + \left(\hat{T} - \frac{\partial\hat{e}}{\partial v}I\right) : D\mathbf{v} - \frac{1}{\theta}\hat{\mathbf{q}} \cdot D\theta. \tag{6}$$

The main point is that (6) must hold for *all* admissible thermodynamic processes, and here is how we can build them. First we select any deformation $\boldsymbol{\chi}$ as in §A and any function s. Then $\mathbf{v} = \frac{\partial\boldsymbol{\chi}}{\partial t}$, $F = D_X\boldsymbol{\chi}$, $\rho = (\det F)^{-1}\rho_0$. Thus we have $v = \rho^{-1}$ and so can then employ

(2) to compute $e, \theta, \mathbf{T}, \mathbf{q}$. Lastly the balance of momentum and energy equations ((2), (4) from §B) allow us to *define* $\mathbf{b}, r$.

We as follows exploit this freedom in choosing $\boldsymbol{\chi}, s$. First fix any time $t_0 > 0$. Then choose $\boldsymbol{\chi}$ as above so that $\rho(\cdot, t_0) = (\det F(\cdot, t_0))^{-1}\rho_0 \equiv \rho$ is constant, and s so that $s(\cdot, t_0) \equiv s$ is constant. Then $v(\cdot, t_0)$ is constant, whence (2)(b) implies $D\theta(\cdot, t_0) = 0$. Fix any point $x_0 \in U(t_0)$. We can choose $\boldsymbol{\chi}, s$ as above, so that $D\mathbf{v} = L = \frac{\partial F}{\partial t}F^{-1}$ and $\frac{Ds}{Dt}$ at (x_0, t_0) are arbitrary. As (6) implies

$$0 \leq \rho\left(\hat{\theta} - \frac{\partial \hat{e}}{\partial s}\right)\frac{Ds}{Dt} + \left(\hat{T} - \frac{\partial \hat{e}}{\partial v}I\right) : D\mathbf{v}$$

at (x_0, t_0) for all choices of $D\mathbf{v}$, $\frac{Ds}{Dt}$, we conclude $\hat{\theta} = \frac{\partial \hat{e}}{\partial s}$, $\hat{T} = \frac{\partial \hat{e}}{\partial v}I$. We rewrite these formulas, dropping the circumflex:

$$\frac{\partial e}{\partial s} = \theta \qquad \textit{temperature formula} \tag{7}$$

and

$$\mathbf{T} = -pI, \tag{8}$$

for

$$\frac{\partial e}{\partial v} = -p \qquad \textit{pressure formula.} \tag{9}$$

Equation (9) is the definition of the pressure $p = \hat{p}(s, v)$. Thus in (7)–(9) we regard $e, \mathbf{T}, p$ as functions of (s, v).

Remarks. (i) The balance of momentum equation (for $\mathbf{b} \equiv 0$) becomes the *compressible Euler equations*

$$\rho\frac{Dv}{Dt} = -Dp, \tag{10}$$

about which more later. If the flow is incompressible, then ρ is constant (say $\rho \equiv 1$) and thus (6) in §A implies div $\mathbf{v} = 0$. We obtain then the *incompressible Euler equations*

$$\begin{cases} \frac{D\mathbf{v}}{Dt} &= -Dp \\ \text{div } \mathbf{v} &= 0. \end{cases} \tag{11}$$

(ii) Note the similarity of (7), (9) with the classical formulas

$$\frac{\partial E}{\partial S} = T, \ \frac{\partial E}{\partial V} = -P$$

for a simple fluid in Chapter I. □

Returning to (6), we conclude from (7)–(9) that

$$\hat{\mathbf{q}}(s, v, D\theta) \cdot D\theta \leq 0.$$

As s, v, and $D\theta$ are arbitrary, provided $D\hat{\theta}(s, v) \neq 0$, we deduce:

$$q(s, v, p) \cdot p \leq 0 \qquad \textit{heat conduction inequality} \tag{12}$$

for all s, v and all $p \in \mathbb{R}^n$. Since the mapping

$$p \mapsto \hat{\mathbf{q}}(s, v, p) \cdot p$$

has a maximum at $p = 0$, we see as well that

$$\hat{\mathbf{q}}(s, v, 0) = 0,$$

which means *there is no heat flow without a temperature gradient.*

b. We call our body a *viscous fluid with heat conduction* if there exist five functions $\hat{e}, \hat{\theta}, \hat{\mathbf{T}}, \hat{l}, \hat{\mathbf{q}}$ such that

$$\begin{cases} \text{(a)} & e = \hat{e}(s, v) \\ \text{(b)} & \theta = \hat{\theta}(s, v) \\ \text{(c)} & \mathbf{T} = \hat{\mathbf{T}}(x, v) + \hat{l}(s, v)[D\mathbf{v}] \\ \text{(d)} & \mathbf{q} = \hat{\mathbf{q}}(s, v, D\theta). \end{cases} \tag{13}$$

Here for each (s, v), we assume $\hat{l}(s, v)[\cdot]$ is a linear mapping from $\mathbb{M}^{3\times 3}$ into $\mathbb{S}^3$. This term models the fluid viscosity.

As before, we conclude from the Clausius–Duhem inequality that

$$0 \leq \rho \left(\hat{\theta} - \frac{\partial \hat{e}}{\partial s} \right) \frac{Ds}{Dt} + \left(\hat{T} - \frac{\partial \hat{e}}{\partial v} I \right) : D\mathbf{v} + \hat{l}[D\mathbf{v}] : D\mathbf{v} - \frac{1}{\theta} \hat{q} \cdot D\theta.$$

Since this estimate must be true for all $\boldsymbol{\chi}$ and s, we deduce as before the temperature formula (7).

We then pick $\boldsymbol{\chi}, s$ appropriately to deduce:

$$0 \leq \left(\hat{T} - \frac{\partial \hat{e}}{\partial v} I \right) : D\mathbf{v} + \hat{l}[D\mathbf{v}] : D\mathbf{v}.$$

In this expression $D\mathbf{v}$ is arbitrary, and so in fact

$$0 \leq \lambda \left(\hat{T} - \frac{\partial \hat{e}}{\partial v} I \right) : D\mathbf{v} + \lambda^2 \hat{l}[D\mathbf{v}] : D\mathbf{v}$$

for each $\lambda \in \mathbb{R}$. If we define $\hat{p}$ by (9), the identity

$$\mathbf{T} = -pI + l[Dv] \tag{14}$$

follows, as does the inequality

$$l(L) : L \geq 0 \qquad \textit{dissipation inequality} \tag{15}$$

for all $L \in \mathbb{M}^{3\times 3}$. The heat conduction inequality (12) then results.

Remark. As explained in [C-N] constitutive relations must also satisfy the *principle of material objectivity*, which means that an admissible process must remain so after a (possibly time dependent) orthogonal change of frame. This principle turns out to imply that $l[\cdot]$ must have the form

$$l[D\mathbf{v}] = \mu(D\mathbf{v} + (D\mathbf{v})^T) + \lambda(\text{div } \mathbf{v})I \tag{16}$$

where μ, λ are scalar functions of (s, v). The dissipative inequality (15) turns out to force

$$\mu \geq 0, \ \lambda + \frac{2}{3}\mu \geq 0.$$

Taking μ, λ to be constant in the balance of motion equations (for $\mathbf{b} \equiv 0$) gives the *compressible Navier–Stokes equations*

$$\rho \frac{D\mathbf{v}}{Dt} = -Dp + \mu\Delta\mathbf{v} + (\lambda + \mu)D(\text{div } \mathbf{v}). \tag{17}$$

If the flow is *incompressible*, then ρ is constant (say $\rho \equiv 1$) and so the conservation of momentum equation implies div $\mathbf{v} \equiv 0$. We thereby derive the *incompressible Navier–Stokes equations*

$$\begin{cases} \frac{D\mathbf{v}}{Dt} &= -Dp + \mu\Delta\mathbf{v} \\ \text{div } \mathbf{v} &= 0. \end{cases} \tag{18}$$

□

2. Elastic materials

We can also model as well elastic solids, for which it is appropriate to display certain quantities in Lagrangian coordinates (i.e., in terms of X, not x).

a. We call our body a *perfect elastic material with heat conduction* provided there exist four functions $\hat{e}, \hat{\theta}, \hat{\mathbf{T}}, \hat{\mathbf{q}}$ such that

$$\begin{cases} \text{(a)} & e = \hat{e}(s, F) \\ \text{(b)} & \theta = \hat{\theta}(s, F) \\ \text{(c)} & \mathbf{T} = \hat{\mathbf{T}}(s, F) \\ \text{(d)} & \mathbf{q} = \hat{\mathbf{q}}(s, F, D\theta). \end{cases} \tag{19}$$

These are the *constitutive relations*.

Notation. Equation (a) means

$$e(x,t) = \hat{e}(s(x,t), F(X,t)) \qquad (x \in U(t),\ t \geq 0)$$

where $\hat{e} : \mathbb{M}^{3\times 3} \times \mathbb{R} \to \mathbb{R}$ and $X = \boldsymbol{\psi}(x,t)$. Equations (b)–(d) have similar interpretations. Recall from §A that $F = D_X \boldsymbol{\chi}$ is the deformation gradient. □

According to (3):

$$0 \leq \rho\left(\theta \frac{Ds}{Dt} - \frac{De}{Dt}\right) + \mathbf{T} : D\mathbf{v} - \frac{1}{\theta}\mathbf{q} \cdot D\theta. \tag{20}$$

Owing to (19)(a) we have

$$\frac{De}{Dt} = \frac{\partial \hat{e}}{\partial s}\frac{Ds}{Dt} + \frac{\partial \hat{e}}{\partial F} : \left[\frac{\partial F}{\partial t} + D_X F \cdot \frac{D\psi}{Dt}\right]^{2}.$$

Differentiate the identity $\boldsymbol{\psi}(\boldsymbol{\chi}(X,t),t) = X$ with respect to t, to deduce $\frac{D\boldsymbol{\psi}}{Dt} = 0$. So

$$\frac{De}{Dt} = \frac{\partial \hat{e}}{\partial s}\frac{Ds}{Dt} + \frac{\partial \hat{e}}{\partial F} : \frac{\partial F}{\partial t}.$$

Recalling from (9), (10) in §A that $D\mathbf{v} = L = \frac{\partial F}{\partial t}F^{-1}$, we substitute into (20), thereby deducing

$$0 \leq \rho\left(\hat{\theta} - \frac{\partial \hat{e}}{\partial s}\right)\frac{Ds}{Dt} + \left(\hat{\mathbf{T}} - \rho\frac{\partial \hat{e}}{\partial F}F^{T}\right) : D\mathbf{v} - \frac{1}{\theta}\hat{\mathbf{q}} \cdot D\theta. \tag{21}$$

Fix $t_0 > 0$. We take $\boldsymbol{\chi}$ so that $D_X\boldsymbol{\chi}(\cdot, t_0) = F(\cdot, t_0) = F$, an arbitrary matrix. Next we pick s so that $s(\cdot, 0) \equiv s$ is constant. Thus (19)(b) forces $D\theta(\cdot, 0) = 0$. As $D\mathbf{v} = L = \frac{\partial F}{\partial t}F^{-1}$ and $\frac{Ds}{Dt}$ can take any values at $t = t_0$, we deduce from (21) the temperature formula (7), as well as the identity

$$T = \rho\frac{\partial e}{\partial F}F^{T} \qquad \textit{stress formula,} \tag{22}$$

where, we recall from (11) in §A, $\rho = (\det F)^{-1}\rho_0$. Here we have again dropped the circumflex, as so are regarding T, e as functions of (s, F). Next the heat conduction inequality (12) follows as usual.

[2] In coordinates: $\left(\frac{\partial \hat{e}}{\partial F}\right)_{ij} = \frac{\partial \hat{e}}{\partial F_{ij}}$, $(1 \leq i, j \leq 3)$.

Note. Let us check that (22) reduces to (8), (9) in the case of a fluid, i.e. $\hat{e} = \hat{e}(s, v)$, $v = \rho^{-1} = (\det\ F)\rho_0^{-1}$. Then the (i, j)-th entry of $\hat{T}$ is

$$\rho \sum_{k=1}^{3} \frac{\partial \hat{e}}{\partial F_{ik}} F_{jk} = \frac{\rho}{\rho_0} \frac{\partial \hat{e}}{\partial v} \sum_{k=1}^{3} \frac{\partial(\det\ F)}{\partial F_{ik}} F_{jk}.$$

Now

$$\frac{\partial(\det\ F)}{\partial F_{ik}} = (\text{cof}\ F)_{ik},$$

cof F denoting the cofactor matrix of F. Thus

$$\begin{aligned} \hat{T} = \rho \tfrac{\partial \hat{e}}{\partial F} F^T &= \tfrac{\rho}{\rho_0} \tfrac{\partial \hat{e}}{\partial v} (\text{cof}\ F) F^T \\ &= \tfrac{\rho}{\rho_0} \tfrac{\partial \hat{e}}{\partial v} (\det\ F) I. \end{aligned}$$

As $\rho = (\det\ F)^{-1}\rho_0$, we conclude $\hat{T} = \frac{\partial \hat{e}}{\partial v} I$, and this identity is equivalent to (8), (9). □

b. We have a *viscous elastic material with heat conduction* if these constitutive relations hold:

$$(23) \qquad \begin{cases} \text{(a)} & e = \hat{e}(s, F) \\ \text{(b)} & \theta = \hat{\theta}(s, F) \\ \text{(c)} & \mathbf{T} = \hat{\mathbf{T}}(s, F) + \hat{l}(s, F)[D\mathbf{v}] \\ \text{(d)} & \mathbf{q} = \hat{\mathbf{q}}(s, F, D\theta). \end{cases}$$

We deduce as above the temperature formula (7), the heat conduction inequality (12), the dissipation inequality (15), and the identity

$$\mathbf{T} = \rho \frac{\partial e}{\partial F} F^T + l[D\mathbf{v}].$$

Remark. Our constitutive rules (2), (13), (19), (23) actually violate the general *principle of equipresence*, according to which a quantity present in an independent variable in one constitutive equation should be present in all, unless its presence contradicts some rule of physics or an invariance rule. See Truesdell–Noll [T-N, p. 359–363] for an analysis incorporating this principle.

D. Workless dissipation

Our model from §II.A of a homogeneous fluid body without dissipation illustrated an idealized physical situation in which work, but not dissipation, can occur. This is *dissipationless work*. We now provide a mathematical framework for *workless dissipation* (from Gurtin [GU, Chapter 14]).

We adopt the terminology from §A–C above, with the additional proviso that our material body is now assumed to be *rigid*. So $U(t) = U(\text{for all } t \geq 0)$ and

$$\mathbf{v} \equiv 0, \ \mathbf{b} \equiv 0. \tag{1}$$

We simplify further by supposing the mass density is constant:

$$\rho \equiv 1. \tag{2}$$

The remaining relevant physical quantities are thus $e, \mathbf{q}, r, s$ and θ.

Under assumption (1) the momentum balance equation is trivial. The energy balance equation ((4) in §B) now reads:

$$\frac{\partial e}{\partial t} = r - \ \text{div}\ \mathbf{q} \tag{3}$$

and the entropy flux inequality ((6) in §B) becomes:

$$\frac{\partial s}{\partial t} \geq \frac{r}{\theta} - \ \text{div}\left(\frac{\mathbf{q}}{\theta}\right). \tag{4}$$

The *local production of entropy* is

$$\gamma = \frac{\partial s}{\partial t} - \frac{r}{\theta} + \frac{\text{div}(\mathbf{q})}{\theta} - \frac{\mathbf{q} \cdot D\theta}{\theta^2} \geq 0. \tag{5}$$

Combining (3)–(5) as before, we deduce:

$$0 \leq \gamma\theta = \left(\theta \frac{\partial s}{\partial t} - \frac{\partial e}{\partial t}\right) - \frac{\mathbf{q} \cdot D\theta}{\theta}. \tag{6}$$

It is convenient to introduce the *free energy*/unit mass:

$$f = e - \theta s, \tag{7}$$

a relation reminiscent of the formula $F = E - TS$ from Chapter 1. In terms of f, (6) becomes:

$$\frac{\partial f}{\partial t} + s\frac{\partial \theta}{\partial t} + \frac{\mathbf{q} \cdot D\theta}{\theta} \leq 0. \tag{8}$$

For our model of *heat conduction in a rigid body* we introduce next the constitutive relations

$$\begin{cases} \text{(a)} & e = \hat{e}(\theta, D\theta) \\ \text{(b)} & s = \hat{s}(\theta, D\theta) \\ \text{(c)} & \mathbf{q} = \hat{\mathbf{q}}(\theta, D\theta) \end{cases} \tag{9}$$

where $\hat{e}, \hat{s}, \hat{\mathbf{q}}$ are given functions. We seek to determine what (8) implies about these structural functions.

First, define

$$\hat{f}(\theta, p) := \hat{e}(\theta, p) - \theta \hat{s}(\theta, p); \tag{10}$$

so that (7) says

$$f = \hat{f}(\theta, D\theta).$$

Therefore

$$\frac{\partial f}{\partial t} = \frac{\partial \hat{f}}{\partial \theta}\frac{\partial \theta}{\partial t} + D_p \hat{f} \cdot D\left(\frac{\partial \theta}{\partial t}\right).$$

Plug into (8):

$$\left(\frac{\partial \hat{f}}{\partial \theta} + \hat{s}\right)\frac{\partial \theta}{\partial t} + D_p \hat{f} \cdot D\left(\frac{\partial \theta}{\partial t}\right) + \frac{\hat{\mathbf{q}} \cdot D\theta}{\theta} \leq 0. \tag{11}$$

As before, we can select θ so that $\frac{\partial \theta}{\partial t}$, $D\left(\frac{\partial \theta}{\partial t}\right)$ and $D\theta$ are arbitrary at any given point (x, t). Consequently we deduce

$$\frac{\partial f}{\partial \theta} = -s \qquad \textit{free energy formula,} \tag{12}$$

an analogue of the classical relation

$$\frac{\partial F}{\partial T} = -S$$

discussed in Chapter I. Also we conclude

$$D_p \hat{f} = 0, \tag{13}$$

and so (10) implies

$$D_p \hat{e}(\theta, p) = \theta D_p \hat{s}(\theta, p)$$

for all θ, p. But (12), (13) allow us to deduce

$$0 = \frac{\partial}{\partial \theta}(D_p \hat{f}) = -D_p \hat{s}.$$

Hence $D_p \hat{e} \equiv D_p \hat{s} \equiv 0$, and so $\hat{e}, \hat{s}$ do not depend on p. Thus (9)(a), (b) become

$$\begin{cases} e = e(\theta) \\ s = s(\theta). \end{cases} \tag{14}$$

The energy and entropy thus depend only on θ and not $D\theta$. Finally we conclude from (11) that

$$\mathbf{q}(\theta, p) \cdot p \leq 0 \qquad \textit{heat conduction inequality} \tag{15}$$

for all θ, p. The free energy is

$$f = \hat{f}(\theta) = \hat{e}(\theta) - \theta \hat{s}(\theta).$$

Finally we define the *heat capacity*/unit mass:

$$c_v(\theta) = e'(\theta), \qquad \left(' = \frac{d}{d\theta}\right), \tag{16}$$

in analogy with the classical formula

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V.$$

Let us compute $\hat{f}' = \hat{e}' - \hat{s} - \theta \hat{s}'$; whence (12), (16) imply

$$-\hat{f}'' = \hat{s}' = \frac{c_v}{\theta}.$$

In summary

$$c_v(\theta) = \theta s'(\theta) = -\theta f(\theta)''. \tag{17}$$

In particular f is a strictly concave function of θ if and only if $c_v(\cdot) > 0$.

Finally we derive from (3), (16) the *general heat conduction equation*

$$c_v(\theta)\frac{\partial \theta}{\partial t} + \ \mathrm{div}(\mathbf{q}(\theta, D\theta)) = r. \tag{18}$$

This is a PDE for the temperature $\theta = \theta(x, t)$ $(x \in U,\ t \geq 0)$. The local production of entropy is

$$\gamma = \frac{-\mathbf{q}(\theta, D\theta) \cdot D\theta}{\theta^2} = \mathbf{q}(\theta, D\theta) \cdot D\left(\frac{1}{\theta}\right). \tag{19}$$

Remark. The special case that

$$\mathbf{q}(\theta, p) = -Ap \tag{20}$$

is called *Fourier's Law*, where $A \in \mathbb{M}^{3\times 3}$, $A = ((a_{ij}))$. Owing to the heat conduction inequality, we must then have

$$p \cdot (Ap) \geq 0 \text{ for all } p,$$

and so

$$\sum_{i,j=1}^{3} a_{ij}\xi_i\xi_j \geq 0 \qquad (\xi \in \mathbb{R}^3). \tag{21}$$

□

CHAPTER 4: Elliptic and parabolic equations

In this chapter we will analyze linear PDE of elliptic and parabolic type in light of the physical theory set forth in Chapters I–III above. We will mostly follow Day [D].

Generic PDE notation.

$$\begin{aligned} U, V, W &= \text{open subsets, usually of } \mathbb{R}^n \\ u, v, w &= \text{typical functions} \\ u_t &= \tfrac{\partial u}{\partial t},\ u_{x_i} = \tfrac{\partial u}{\partial x_i},\ u_{x_i x_j} = \tfrac{\partial^2 u}{\partial x_i \partial x_j},\ \text{etc.} \end{aligned}$$

□

A. Entropy and elliptic equations

1. Definitions

We will first study the linear PDE

$$-\sum_{i,j=1}^{n} (a^{ij}(x) u_{x_i})_{x_j} = f \text{ in } U, \tag{1}$$

where $U \subset \mathbb{R}^n$ is a bounded, connected open set with smooth boundary ∂U,

$$f : \bar{U} \to \mathbb{R},$$

and

$$A : \bar{U} \to \mathbb{S}^n,\ A = ((a^{ij})).$$

The unknown is

$$u = u(x) \qquad (x \in \bar{U}).$$

We assume $u > 0$ in $\bar{U}$ and u is smooth.

Physical interpretation. We henceforth regard (1) as a time-independent *heat conduction* PDE, having the form of (18) from §III.D, with

$$\begin{cases} u &= \text{temperature} \\ \mathbf{q} &= -ADu = \text{ heat flux} \\ f &= \text{heat supply/unit mass.} \end{cases} \tag{2}$$

We will additionally assume in the heat condition PDE that the heat capacity c_v is a constant, say $c_v \equiv 1$. Then, up to additive constants, we see from formula (17) in §III.D that

$$\begin{cases} u &= \text{internal energy/unit mass} \\ \log u &= \text{entropy/unit mass.} \end{cases} \tag{3}$$

The *local production of entropy* is

$$\gamma = \sum_{i,j=1}^{n} a^{ij} \frac{u_{x_i} u_{x_j}}{u^2}. \tag{4}$$

We will henceforth assume the PDE (1) is *uniformly elliptic*, which means that there exists a positive constant θ such that

$$\sum_{i,j=1}^{n} a^{ij}(x)\xi_i\xi_j \geq \theta|\xi|^2 \tag{5}$$

for all $x \in \bar{U}$, $\xi \in \mathbb{R}^n$. We assume as well that the coefficient functions $\{a^{ij}\}_{i,j=1}^n$ are smooth. Note that (5) implies $\gamma \geq 0$.

Notation. (i) If V is any smooth region, the outer unit normal vector field is denoted $\boldsymbol{\nu} = (\nu_1, \ldots, \nu_n)$. The *outer A-normal field* is

$$\boldsymbol{\nu}_A = A\boldsymbol{\nu}. \tag{6}$$

(ii) If $u : \bar{V} \to \mathbb{R}$ is smooth, the *A-normal derivative* of u on ∂V is

$$\frac{\partial u}{\partial \nu_A} = Du \cdot (A\boldsymbol{\nu}) = \sum_{i,j=1}^{n} a^{ij}\nu_i u_{x_j}. \tag{7}$$

□

Note. According to (5) $\boldsymbol{\nu}_A \cdot \boldsymbol{\nu} > 0$ on ∂V and so $\boldsymbol{\nu}_A$ is an outward pointing vector field.

□

Definitions. Let $V \subset U$ be any smooth region. We define

$$F(V) = \int_V \frac{f}{u} dx = \textit{ entropy supply to } V \tag{8}$$

$$G(V) = \int_V \gamma dx = \int_V \sum_{i,j=1}^{n} \frac{a^{ij} u_{x_i} u_{x_j}}{u^2} dx = \textit{ internal entropy production} \tag{9}$$

(10) $$R(V) = -\int_{\partial V} \frac{1}{u}\frac{\partial u}{\partial \nu_A} dS = \text{ } \textit{entropy flux} \text{ outward across } \partial V.$$

Lemma *For each subregion $V \subset U$, we have*:

(11) $$F(V) + G(V) = R(V).$$

This is the *entropy balance equation*.

Proof. Divide the PDE (1) by u and rewrite:

$$-\sum_{i,j=1}^n \left(a^{ij}\frac{u_{x_i}}{u}\right)_{x_j} = \sum_{i,j=1}^n \frac{a^{ij}u_{x_i}u_{x_j}}{u^2} + \frac{f}{u}.$$

Integrate over V and employ the Gauss–Green Theorem:

$$\underbrace{-\int_{\partial V} \frac{1}{u}\sum_{i,j=1}^n a^{ij}u_{x_i}\nu_j dS}_{R(V)} = \underbrace{\int_V \sum_{i,j=1}^n a^{ij}\frac{u_{x_i}u_{x_j}}{u^2}dx}_{G(V)} + \underbrace{\int_V \frac{f}{u}dx}_{F(V)}.$$

□

We henceforth assume

(12) $$f \geq 0 \text{ in } U,$$

meaning physically that only heating is occurring.

2. Estimates of equilibrium entropy production

The PDE (1) implies for each region $V \subset U$ that

(13) $$\int_{\partial V} \mathbf{q}\cdot\boldsymbol{\nu} dS = \int_V f dx$$

for $\mathbf{q} = -ADu$. This equality says that the heat flux outward through ∂V balances the heat production within V. Likewise the identity (11) says

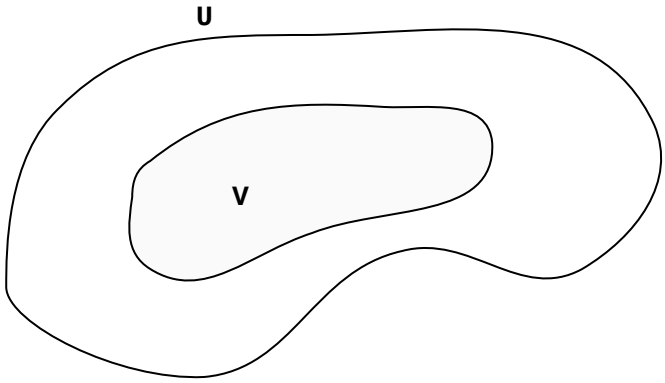
(14) $$\int_V \frac{\mathbf{q}}{\mathbf{u}}\cdot\boldsymbol{\nu} dS = \int_V \gamma + \frac{f}{u}dx,$$

which means the entropy flux outward through ∂V balances the entropy production within V, the later consisting of

$$\int_V \gamma dx, \text{ the rate of internal entropy generation, and}$$
$$\int_V \frac{f}{u} dx, \text{ the entropy supply.}$$

a. A capacity estimate

Now (13) shows clearly that the heat flux outward through ∂U can be made arbitrarily large if we take f large enough. In contrast if $V \subset\subset U$, there is a bound on the size of the entropy flux and the rate of internal entropy production, valid no matter how large f is.



Assume that $V \subset\subset U$ and let w solve the boundary value problem

$$\text{(15)} \qquad \begin{cases} -\sum_{i,j=1}^n (a^{ij}(x) w_{x_i})_{x_j} = 0 & \text{in } U - \bar{V} \\ w = 1 & \text{on } \partial V \\ w = 0 & \text{on } \partial U. \end{cases}$$

Definition. We define the *capacity* of V (with respect to ∂U and the matrix A) to be

$$\text{(16)} \qquad \text{Cap}_A(V, \partial U) = \int_{U-V} \sum_{i,j=1}^n a^{ij} w_{x_i} w_{x_j} dx,$$

w solving (15).

Integrating by parts shows:

$$\text{(17)} \qquad \text{Cap}_A(V, \partial U) = \int_{\partial V} -\frac{\partial w}{\partial \nu_A} dS,$$

ν_A denoting the outer A-normal vector field to V.

Theorem 1 *We have*

$$R(V) \leq \ \mathrm{Cap}_A(V, \partial U) \tag{18}$$

for all choices of $f \geq 0$.

Proof. Take w as in (15) and compute in $U - \bar{V}$:

$$\begin{aligned}
&\textstyle\sum_{i,j=1}^n \left(\frac{w^2}{u} a^{ij} u_{x_i}\right)_{x_j} \\
&\quad = \textstyle\sum_{i,j=1}^n \Big[\frac{w^2}{u}(a^{ij}u_{x_i})_{x_j} - \frac{w^2}{u^2} a^{ij} u_{x_i} u_{x_j} \\
&\qquad + 2\frac{w}{u} a^{ij} u_{x_i} w_{x_j}\Big] \\
&\quad = -\frac{w^2 f}{u} - \textstyle\sum_{i,j=1}^n a^{ij} \left(\frac{w}{u} u_{x_i} - w_{x_i}\right)\left(\frac{w}{u} u_{x_j} - w_{x_j}\right) \\
&\qquad + \textstyle\sum_{i,j=1}^n a^{ij} w_{x_i} w_{x_j},
\end{aligned}$$

where we employed the PDE (1). Since $f \geq 0$ and the elliptivity condition (5) holds, we deduce

$$\sum_{i,j=1}^n \left(\frac{w^2}{u} a^{ij} u_{x_i}\right)_{x_j} \leq \sum_{i,j=1}^n a^{ij} w_{x_i} w_{x_j} \text{ in } U - \bar{V}.$$

Integrate over $U - \bar{V}$:

$$-\int_{\partial V} \frac{w^2}{u} \frac{\partial u}{\partial \nu_A} dS \leq \int_{U-V} \sum_{i,j=1}^n a^{ij} w_{x_i} w_{x_j} dx.$$

Since $w = 1$ on V, the term on the left is $R(V)$, whereas by the definition (16) the term on the right is $\mathrm{Cap}_A(V, \partial U)$. □

Note that the entropy balance equation and (18) imply:

$$G(V) \leq \ \mathrm{Cap}_A(V, \partial U) \tag{19}$$

for all f, the term on the right depending solely on A and the geometry of V, U. The above calculation is from Day [D].

b. A pointwise bound

Next we demonstrate that in fact we have an internal pointwise bound on γ within any region $V \subset\subset U$, provided

$$f \equiv 0 \text{ in } U. \tag{20}$$

Theorem 2 *Assume $f \equiv 0$ in U and $V \subset\subset U$. Then there exists a constant C, depending only on dist$(V, \partial U)$ and the coefficients, such that*

$$\sup_V \gamma \leq C \tag{21}$$

for all positive solutions of (1).

In physical terms, if the heat supply is zero, we can estimate the local production of entropy pointwise within V, completely irrespective of the boundary conditions for the temperature on ∂U.

The following calculation is technically difficult, but—as we will see later in §VIII.D—is important in other contexts as well.

Proof. 1. Let

$$v = \log u \tag{22}$$

denote the entropy. Then the PDE

$$-\sum_{i,j=1}^n (a^{ij} u_{x_i})_{x_j} = 0 \text{ in } U$$

becomes

$$-\sum_{i,j=1}^n (a^{ij} v_{x_i})_{x_j} = \sum_{i,j=1}^n a^{ij} v_{x_i} v_{x_j} = \gamma. \tag{23}$$

So

$$-\sum_{i,j=1}^n a^{ij} v_{x_i x_j} + \sum_{i=1}^n b^i v_{x_i} = \gamma \text{ in } U \tag{24}$$

for

$$b^i := -\sum_{i,j=1}^n a^{ij}_{x_j} \qquad (1 \leq i \leq n).$$

Differentiate (24) with respect to x_k:

$$-\sum_{i,j=1}^n a^{ij} v_{x_k x_i x_j} + \sum_{i=1}^n b^i v_{x_k x_j} = \gamma_{x_k} + R_1, \tag{25}$$

where R_1 denotes an expression satisfying the estimate

$$|R_1| \leq C(|D^2 v| + |Dv|). \tag{26}$$

2. Now

$$\gamma = \sum_{k,l=1}^{n} a^{kl} v_{x_k} v_{x_l}.$$

Thus

$$\left\{ \begin{array}{rcl} \gamma_{x_i} & = & \sum_{k,l=1}^{n} 2a^{kl} v_{x_k x_i} v_{x_l} + a_{kl,x_i} v_{x_k} v_{x_l}, \\ \gamma_{x_i x_j} & = & \sum_{k,l=1}^{n} 2a^{kl} v_{x_k x_i x_j} v_{x_l} + 2a^{kl} v_{x_k x_i} v_{x_l x_j} + R_2, \end{array} \right. \tag{27}$$

where

$$|R_2| \leq C(|D^2 v| \ |Dv| + |Dv|^2). \tag{28}$$

Hence

$$\begin{array}{l} -\sum_{i,j=1}^{n} a^{ij} \gamma_{x_i x_j} + \sum_{i=1}^{n} b^i \gamma_{x_i} \\ \quad = 2 \sum_{k,l=1}^{n} a^{kl} v_{x_l} \left(-\sum_{i,j=1}^{n} a^{ij} v_{x_k x_i x_j} + \sum_{i=1}^{n} b^i v_{x_k x_i} \right) \\ \qquad -2 \sum_{i,j,k,l=1}^{n} a^{ij} a^{kl} v_{x_k x_i} v_{x_l x_j} + R_3, \end{array} \tag{29}$$

R_3 another remainder term satisfying an estimate like (28). In view of the uniform ellipticity condition (5), we have

$$\sum_{i,j,k,l=1}^{n} a^{ij} a^{kl} v_{x_k x_i} v_{x_l x_j} \geq \theta^2 |D^2 v|^2.$$

This estimate and the equality (25) allow us to deduce from (29) that

$$-\sum_{i,j=1}^{n} a^{ij} \gamma_{x_i x_j} + \sum_{i=1}^{n} b^i \gamma_{x_i} \leq 2 \sum_{k,l=1}^{n} a^{kl} v_{x_l} \gamma_{x_k} - 2\theta^2 |D^2 v|^2 + R_4, \tag{30}$$

R_4 satisfying an estimate like (28):

$$|R_4| \leq C(|D^2 v| \ |Dv| + |Dv|^2).$$

Recall now *Cauchy's inequality with* ε

$$ab \leq \varepsilon a^2 + \frac{1}{4\varepsilon} b^2 \qquad (a, b, \varepsilon > 0),$$

and further note

$$\gamma \geq \theta |Dv|^2.$$

Thus

$$|R_4| \leq \theta^2 |D^2 v|^2 + C\gamma.$$

Consequently (30) implies

$$\theta^2|D^2v|^2 - \sum_{i,j=1}^n a^{ij}\gamma_{x_ix_j} \leq C(1+\gamma^{1/2})|D\gamma| + C\gamma. \tag{31}$$

Next observe that the PDE (24) implies

$$\begin{aligned} \gamma &\leq C(|D^2v| + |Dv|) \\ &\leq C(|D^2v| + \gamma^{1/2}) \\ &\leq C|D^2v| + C + \tfrac{\gamma}{2}, \end{aligned}$$

where we again utilized Cauchy's inequality. Thus

$$\gamma \leq C(|D^2v| + 1). \tag{32}$$

This estimate incorporated into (31) yields:

$$\sigma\gamma^2 - \sum_{i,j=1}^n a^{ij}\gamma_{x_ix_j} \leq C(1+\gamma^{1/2})|D\gamma| + C \tag{33}$$

for some $\sigma > 0$.

3. We have managed to show that γ satisfies within U the differential inequality (33), where the positive constants C, σ depend only on the coefficients. Now we demonstrate that this estimate, owing to the quadratic term on the left, implies a bound from above for γ on any subregion $V \subset\subset U$.

So take $V \subset\subset U$ and select a cutoff function $\zeta : U \to \mathbb{R}$ satisfying

$$\begin{cases} 0 \leq \zeta \leq 1, \ \zeta \equiv 1 \text{ on } V, \\ \zeta \equiv 0 \text{ near } \partial U. \end{cases} \tag{34}$$

Write

$$\eta := \zeta^4\gamma \tag{35}$$

and compute

$$\begin{cases} \eta_{x_i} = \zeta^4\gamma_{x_i} + 4\zeta^3\zeta_{x_i}\gamma \\ \eta_{x_ix_j} = \zeta^4\gamma_{x_ix_j} + 4\zeta^3(\zeta_{x_j}\gamma_{x_i} + \zeta_{x_i}\gamma_{x_j}) + 4(\zeta^3\zeta_{x_i})_{x_j}\gamma. \end{cases} \tag{36}$$

Select a point $x_0 \in \bar{U}$, where η attains its maximum. If $\zeta(x_0) = 0$, then $\eta = 0$. Otherwise $\zeta(x_0) > 0$, $x_0 \in U$, and so

$$D\eta(x_0) = 0, \ D^2\eta(x_0) \leq 0.$$

Consequently

$$\zeta D\gamma = -4\gamma D\zeta \text{ at } x_0. \tag{37}$$

So at the point x_0:

$$\begin{aligned} 0 &\leq -\sum_{i,j=1}^n a^{ij}\eta_{x_i x_j} \\ &= -\zeta^4 \sum_{i,j=1}^n a^{ij}\gamma_{x_i x_j} + R_5, \end{aligned}$$

where

$$|R_5| \leq C(\zeta^3|D\gamma| + \zeta^2\gamma). \tag{38}$$

Invoking (33) we compute

$$\sigma\zeta^4\gamma^2 \leq C\zeta^4\gamma^{1/2}|D\gamma| + C + R_6, \tag{39}$$

R_6 being estimated as in (38). Now (37) implies

$$\begin{aligned} \zeta^4\gamma^{1/2}|D\gamma| &\leq C\zeta^3\gamma^{3/2} \\ &\leq \tfrac{\sigma}{4}\zeta^4\gamma^2 + C, \end{aligned}$$

where we employed *Young's inequality with* ε

$$ab \leq \varepsilon a^p + C(\varepsilon)b^q \qquad \left(\frac{1}{p} + \frac{1}{q} = 1,\ a, b, \varepsilon > 0\right)$$

for $p = \frac{4}{3}$, $q = 4$. Also

$$\begin{aligned} |R_6| &\leq C(\zeta^3|D\gamma| + \zeta^2\gamma) \\ &\leq C\zeta^2\gamma \\ &\leq \tfrac{\sigma}{4}\zeta^4\gamma^2 + C. \end{aligned}$$

These estimates and (39) imply

$$\zeta^4\gamma^2 \leq C \text{ at } x_0, \tag{40}$$

the constants C, σ depending only on ζ and the coefficients of the PDE. As $\eta = \zeta^4\gamma$ attains its maximum over $\bar{U}$ at x_0, (40) provides a bound on η.

In particular then, since $\zeta \equiv 1$ on V, estimate (21) follows. □

3. Harnack inequality

As earlier noted, the pointwise estimate (21) is quite significant from several viewpoints. As a first illustration we note that (21) implies

Theorem 3 *For each connected region $V \subset\subset U$ there exists a constant C, depending only on U, V, and the coefficients, such that*

$$\sup_V u \leq C \inf_V u \tag{41}$$

for each nonnegative solution u of

$$-\sum_{i,j=1}^{n} (a^{ij} u_{x_i})_{x_j} = 0 \text{ in } U. \tag{42}$$

Remark. Estimate (41) is *Harnack's inequality* and is important since it is completely independent of the boundary values of u on ∂U. □

Proof. Take $V \subset\subset W \subset\subset U$ and $r > 0$ so small that $B(x,r) \subset W$ for each $x \in V$. Let $\varepsilon > 0$. Since $\tilde{u} = u + \varepsilon > 0$ solves (42), Theorem 2 implies

$$\sup_W \frac{|Du|}{u + \varepsilon} \leq C \tag{43}$$

for some constant C depending only on W, U, etc. Take any points $y, z \in B(x,r) \subset W$. Then

$$\begin{aligned} &|\log(u(y) + \varepsilon) - \log(u(z) + \varepsilon)| \\ &\quad \leq \sup_{B(x,r)} |D \log(u + \varepsilon)| \ |y - z| \\ &\quad \leq 2Cr =: C_1 \end{aligned}$$

owing to (43). So

$$\log(u(y) + \varepsilon) \leq C_1 + \log(u(z) + \varepsilon)$$

and thus

$$u(y) + \varepsilon \leq C_2(\log(u(z) + \varepsilon)$$

for $C_2 := e^{C_1}$. Let $\varepsilon \to 0$ to deduce:

$$\max_{B(x,r)} u \leq C_2 \min_{B(x,r)} u. \tag{44}$$

As V is connected, we can cover V by finitely many overlapping balls $\{B(x_i, r)\}_{i=1}^N$. We repeatedly apply (44), to deduce (41), with $C := C_2^N$. □

Corollary (Strong Maximum Principle) *Assume $u \in C^2(\bar{U})$ solves the* PDE (42)*, and U is bounded, connected. Then either*

$$\min_{\partial U} u < u(x) < \max_{\partial U} u \qquad (x \in U) \tag{45}$$

or else

$$u \text{ is constant on } U. \tag{46}$$

Proof. 1. Take $M := \max_{\partial U} u$, $\tilde{u} = M - u$. Then

$$\begin{cases} -\sum_{i,j=1}^n (a^{ij}\tilde{u}_{x_i})_{x_j} &= 0 \quad \text{in } U \\ \tilde{u} &\geq 0 \quad \text{on } \partial U. \end{cases} \tag{47}$$

Multiply the PDE by $\tilde{u}^-$ and integrate by parts:

$$\theta \int_{U \cap \{\tilde{u}<0\}} |D\tilde{u}|^2 dx \leq -\sum_{i,j=1}^n \int_U a^{ij}\tilde{u}_{x_i}\tilde{u}^-_{x_i} dx = 0. \tag{48}$$

Here we used the fact that

$$D\tilde{u}^- = \begin{cases} 0 & \text{a.e. on } \{\tilde{u} \geq 0\} \\ -D\tilde{u} & \text{a.e. on } \{\tilde{u} < 0\}. \end{cases}$$

Then (48) implies $D\tilde{u}^- = 0$ a.e. in U. As $\tilde{u}^- = 0$ on ∂U, we deduce

$$\tilde{u}^- \equiv 0 \text{ in } U$$

and so

$$\tilde{u} \geq 0 \text{ in } U. \tag{49}$$

This is a form of the *weak maximum principle*.

2. Next take any connected $V \subset\subset U$. Harnack's inequality implies

$$\sup_V \tilde{u} < C \inf_V \tilde{u}.$$

Thus either $\tilde{u} > 0$ everywhere on V or else $\tilde{u} \equiv 0$ on V. This conclusion is true for each V as above: the dichotomy (45), (46) follows. □

Remark. We have deduced Harnack's inequality and thus the strong maximum principle from our interior pointwise bound (21) on the local production of entropy. An interesting philosophical question arises: Are the foregoing *PDE* computations really "entropy calculations" from physics? Purely mathematically the point is that change of variables $v = \log u$ converts the *linear* PDE

$$-\sum_{i,j=1}^n (a^{ij}u_{x_i})_{x_j} = 0 \text{ in } U$$

into the *nonlinear* PDE

$$-\sum_{i,j=1}^{n}(a^{ij}v_{x_i})_{x_j} = \sum_{i,j=1}^{n} a^{ij}, v_{x_i}v_{x_j} \text{ in } U,$$

which owing to the estimate

$$\sum_{i,j=1}^{n} a_{i_j}v_{x_i}v_{x_j} \geq \theta|Dv|^2$$

admits "better than linear" interior estimates. Is all this just a mathematical accident (since log is an important elementary function) or is it an instance of basic physical principles (since entropy is a fundamental thermodynamic concept)? We urgently need a lavishly funded federal research initiative to answer this question. □

B. Entropy and parabolic equations

1. Definitions

We turn our attention now to the time-dependent PDE

$$u_t - \sum_{i,j=1}^{n}(a^{ij}u_{x_i})_{x_j} = f \text{ in } U_T \tag{1}$$

where U is as before and

$$U_T = U \times (0,T]$$

for some $\infty \geq T > 0$. We are given

$$f : \bar{U}_T \to \mathbb{R}$$

and

$$A : \bar{U} \to \mathbb{S}^n \qquad A = ((a^{ij}));$$

and the unknown is

$$u = u(x,t) \qquad (x \in \bar{U},\ 0 \leq t \leq T).$$

We always suppose $u > 0$.

Physical interpretation. We henceforth think of (1) as a heat conduction PDE, having the form of (18) from §III.D with

$$\begin{cases} u &= \text{temperature} \\ \mathbf{q} &= -ADu = \text{ heat flux,} \\ f &= \text{heat supply/unit mass} \end{cases} \tag{2}$$

and the *heat capacity* is taken to be

$$c_v \equiv 1.$$

Also, up to additive constants, we have

$$\text{(3)} \qquad \begin{cases} u &= \text{internal energy/unit mass} \\ \log u &= \text{entropy/unit mass.} \end{cases}$$

The local production of entropy is

$$\gamma = \sum_{i,j=1}^{n} \frac{a^{ij} u_{x_i} u_{x_j}}{u^2}.$$

In the special case that $A = I$, $f \equiv 0$, our PDE (1) reads

$$\text{(4)} \qquad u_t - \Delta u = 0 \text{ in } U_T.$$

This is the *heat equation.* □

Definitions. Let $t \geq 0$ and $V \subset U$ be any smooth subregion. We define

$$\text{(5)} \qquad S(t,V) = \int_V \log u(\cdot,t) dx = \textit{ entropy} \text{ within } V \text{ at time } t$$

$$\text{(6)} \qquad F(t,V) = \int_V \frac{f(\cdot,t)}{u(\cdot,t)} dx = \textit{ entropy supply} \text{ to } V \text{ at time } t$$

$$\text{(7)} \qquad \begin{aligned} G(t,V) = \textstyle\int_V \gamma(\cdot,t) dx &= \textstyle\int_V \sum_{i,j=1}^n a^{ij} \frac{u_{x_i}(\cdot,t) u_{x_j}(\cdot,t)}{u(\cdot,t)^2} dx \\ &= \textit{ rate of internal entropy generation} \text{ in } V \text{ at time } t \end{aligned}$$

$$\text{(8)} \qquad R(t,V) = -\int_{\partial V} \frac{1}{u(\cdot,t)} \frac{\partial u(\cdot,t)}{\partial \nu_A} dS = \textit{ entropy flux} \text{ outward across } \partial V \text{ at time } t.$$

Lemma *For each $t \geq 0$ and each subregion $V \subset U$ we have*

$$\text{(9)} \qquad \frac{d}{dt} S(t,V) = F(t,V) + G(t,V) - R(t,V).$$

This is the *entropy production equation.*

Proof. Divide the PDE (1) by u and rewrite:

$$\frac{u_t}{u} - \left(\sum_{i,j=1}^{n} a^{ij} \frac{u_{x_i}}{u} \right)_{x_j} = \sum_{i,j=1}^{n} a^{ij} \frac{u_{x_i} u_{x_j}}{u^2} + \frac{f}{u}.$$

Integrate over V:

$$\underbrace{\int_V \frac{u_t}{u} dx}_{\frac{d}{dt}S(t,v)} + \underbrace{\int -\frac{1}{u} \frac{\partial u}{\partial \nu_A} dS}_{R(t,V)} = \underbrace{\int_V \gamma dx}_{G(t,V)} + \underbrace{\int_V \frac{f}{u} dx}_{F(t,V).}$$

□

2. Evolution of entropy

In this section we suppose that

$$f \geq 0 \text{ in } U \times (0, \infty) \tag{10}$$

and also

$$\frac{\partial u}{\partial \nu_A} = 0 \text{ on } \partial U \times [0, \infty). \tag{11}$$

The boundary condition (11) means there is no heat flux across ∂U: the boundary is *insulated*.

a. Entropy increase

Define

$$S(t) = \int_U \log u(\cdot, t) dx \qquad (t \geq 0).$$

Theorem 1 *Assume $u \geq 0$ solves* (1) *and conditions* (10), (11) *hold. Then*

$$\frac{dS}{dt} \geq 0 \text{ on } [0, \infty). \tag{12}$$

The proof is trivial: take $V = U$ in the entropy production equation (9) and note that (11) implies $R(t, U) = 0$.

Remarks. (i) Estimate (12) is of course consistent with the physical principle that entropy cannot decrease in any isolated system. But in fact the same proof shows that

$$t \mapsto \int_U \Phi(u(\cdot, t)) dx$$

is nondecreasing, if $\Phi : (0,\infty) \to \mathbb{R}$ is any smooth function with $\Phi' \leq 0$, $\Phi'' \geq 0$. Indeed

$$
\begin{aligned}
\tfrac{d}{dt}\textstyle\int_U \Phi(u)dx &= \textstyle\int_U \Phi'(u)u_t dx \\
&= \textstyle\int_U \Phi'(u)\left[\left(\sum_{i,j=1}^n a^{ij}u_{x_i}\right)_{x_j} + f\right]dx \\
&\leq -\textstyle\int_U \Phi''(u)\sum_{i,j=1}^n a^{ij}u_{x_i}u_{x_j}dx \\
&\leq 0.
\end{aligned} \tag{13}
$$

If $f \equiv 0$, the same conclusion holds if only $\Phi'' \geq 0$, i.e. Φ is convex.

So the entropy growth inequality (12) is just the special case $\Phi(z) = -\log z$ of a general convexity argument. Is there anything particularly special about the physical case $\Phi(z) = -\log z$?

(ii) There is a partial answer, which makes sense physically if we change our interpretation. For simplicity now take $a^{ij} = \delta_{ij}$ and regard the PDE

$$u_t - \Delta u = 0 \text{ in } U \times (0,\infty) \tag{14}$$

as a *diffusion equation*. So now $u = u(x,t) > 0$ represents the *density* of some physical quantity (e.g. a chemical concentration) diffusing within U as time evolves. If $V \subset\subset U$, we hypothesize that

$$\frac{d}{dt}\left(\int_V u(\cdot,t)dx\right) = \int_{\partial V}\frac{\partial u}{\partial \nu}ds \tag{15}$$

which says that the rate of change of the total quantity within V equals the outward flux through ∂V normal to the surface. The identity (15) holding for all $t \geq 0$ and all $V \subset\subset U$, implies u solves the diffusion equation (14).

Next think of the physical quantity (whose density is u) as being passively transported by a flow with velocity field $\mathbf{v} = \mathbf{v}(x,t)$. As in §III.A, we have

$$0 = \frac{d}{dt}\int_{V(t)} u dx = \int_{V(t)} u_t + \text{ div}(u\mathbf{v})dx,$$

$V(t)$ denoting a region moving with the flow. Then

$$u_t + \text{ div}(u\mathbf{v}) = 0. \tag{16}$$

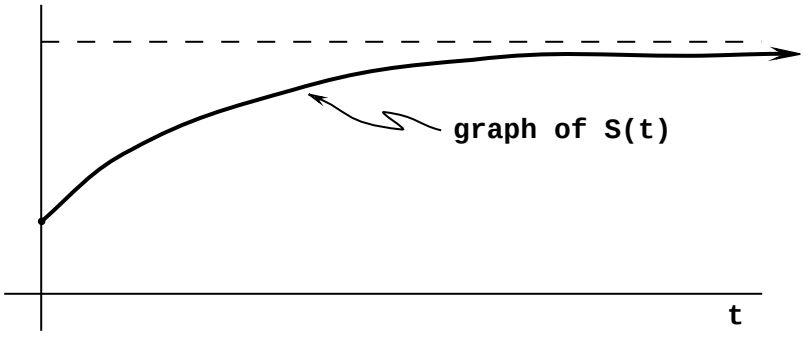
Equations (14), (16) are compatible if

$$\mathbf{v} = -\frac{Du}{u} = -Ds \tag{17}$$

$s = \log u$ denoting the entropy density. So we can perhaps imagine the density as moving microscopically with velocity equaling the *negative* of the gradient of the entropy density. Locally such a motion should tend to *decrease* s, but globally $S(t) = \int_U s(\cdot,t)dx$ *increases*. □

b. Second derivatives in time

Since $\frac{dS}{dt} \geq 0$ and S is bounded, it seems reasonable to imagine the graph of $t \mapsto S(t)$ this way.



We accordingly might conjecture that $t \mapsto S(t)$ is concave and so $\frac{d^2S}{dt^2} \leq 0$ on $[0,\infty)$. This is true in dimension $n = 1$, but false in general: Day in [D, Chapter 5] constructs an example where $n = 2$, U is a square and $\frac{d^2}{dt^2}S(0) > 0$.

We turn our attention therefore to a related physical quantity for which a concavity in time assertion is true. Let us write

$$H(t) = \int_U u(\cdot,t) \log u(\cdot,t)dx. \tag{18}$$

Remark. Owing to (3) we should be inclined to think of $\int_U u(\cdot,t) - u(\cdot,t)\log u(\cdot,t)dx$ as representing the free energy at time t. This is not so good however, as $\Phi(z) = z\log z - z$ is convex and so if $f \equiv 0$, $t \mapsto \int_U u(\cdot,t) - u(\cdot,t)\log u(\cdot,t)dx$ is nondecreasing. This conclusion is physically wrong: the free (a.k.a. available) energy should be diminishing during an irreversible process.

It is worth considering expressions of the form (18) however, as they often appear in the PDE literature under the name "entropy": see e.g. Chow [CB], Hamilton [H], and see also §V.A following. □

Theorem 2 *Assume $u > 0$ solves the heat equation* (14)*, with*

$$\frac{\partial u}{\partial \nu} = 0 \text{ on } \partial U \times [0,\infty).$$

(i) *We have*

$$\frac{dH}{dt} \leq 0 \text{ on } [0,\infty). \tag{19}$$

(ii) *If U is convex, then*

$$\frac{d^2H}{dt^2} \geq 0 \text{ on } [0,\infty). \tag{20}$$

We will need this

Lemma. *Let $U \subset \mathbb{R}^n$ be smooth, bounded, convex. Suppose $u \in C^2(\bar{U})$ satisfies*

$$\frac{\partial u}{\partial \nu} = 0 \text{ on } \partial U. \tag{21}$$

Then

$$\frac{\partial |Du|^2}{\partial \nu} \leq 0 \text{ on } \partial U. \tag{22}$$

Proof. 1. Fix any point x^0 on ∂U. We may without loss assume that $x^0 = 0$ and that near 0, ∂U is the graph in the e_n-direction of a convex function $\gamma : \mathbb{R}^{n-1} \to \mathbb{R}$, with

$$D\gamma(0) = 0 \tag{23}$$

Thus a typical point $x \in \partial U$ near 0 is written as

$$(x', \gamma(x')) \text{ for } x' \in \mathbb{R}^{n-1},\ x' \text{ near } 0.$$

Let h denote any smooth function which vanishes on ∂U. Then

$$h(x', \gamma(x')) \equiv 0 \text{ near } 0.$$

Thus if $i \in \{1, \dots, n-1\}$,

$$h_{x_i} + h_{x_n}\gamma_{x_i} = 0 \text{ near } 0;$$

and consequently

$$h_{x_i}(0) = 0 \qquad (i = 1, \dots, n-1). \tag{24}$$

2. Set $h = \frac{\partial u}{\partial \nu} = \sum_{j=1}^n u_{x_j}\nu^j$, where $\boldsymbol{\nu} = (\nu^1, \dots, \nu^n)$. Then (21), (24) imply

$$\sum_{j=1}^n u_{x_i x_j}\nu^j + u_{x_j}\nu^j_{x_i} = 0 \qquad (i = 1, \dots, n-1) \tag{25}$$

at 0. Now

$$\frac{\partial |Du|^2}{\partial \nu} = 2\sum_{i,j=1}^n u_{x_i}\nu^j u_{x_i x_j},$$

and consequently (25) says

$$\frac{\partial |Du|^2}{\partial \nu} = -2\sum_{i,j=1}^n u_{x_i}u_{x_j}\nu^j_{x_i} \text{ at } 0. \tag{26}$$

3. But since ∂U is the graph of γ near 0, we have

$$\begin{cases} \nu^j = \frac{\gamma_{x_j}}{(1+|D\gamma|^2)^{1/2}} & (j=1,\dots,n-1) \\ \nu^n = \frac{-1}{(1+|D\gamma|^2)^{1/2}}. \end{cases}$$

So for $1 \le i,j \le n-1$:

$$\nu^j_{x_i} = \frac{\gamma_{x_i x_j}}{(1+|D\gamma|^2)^{1/2}} - \sum_{k=1}^{n-1}\frac{\gamma_{x_j}\gamma_{x_k}\gamma_{x_k x_i}}{(1+|D\gamma|^2)^{3/2}}.$$

As (21) implies $u_{x_n}(0)=0$, we conclude from (23), (26) that

$$\frac{\partial |Du|^2}{\partial \nu} = -2\sum_{i,j=1}^{n-1} u_{x_i}u_{x_j}\gamma_{x_i x_j} \le 0 \text{ at } 0,$$

since γ is a convex function. □

Proof of Theorem 2. 1. In light of (18),

$$\begin{aligned} \tfrac{d}{dt}H(t) &= \textstyle\int_U u_t \log u + u\frac{u_t}{u}dx \\ &= \textstyle\int_U \Delta u \log u + \Delta u dx \\ &= \textstyle -\int_U \frac{|Du|^2}{u}dx, \end{aligned}$$

where we used the no-flux boundary condition $\frac{\partial u}{\partial \nu} = 0$ on ∂U.

2. Suppose now U is convex. Then

$$\begin{aligned} \tfrac{d^2}{dt^2}H(t) &= \textstyle\int_U -2\frac{Du\cdot Du_t}{u} + \frac{|Du|^2}{u^2}u_t dx \\ &= \textstyle\int_U -2\sum_{i,j=1}^n \frac{u_{x_i}}{u}u_{x_i x_j x_j} + \sum_{j=1}^n \frac{|Du|^2}{u^2}u_{x_j x_j}dx, \end{aligned}$$

since $u_t = \Delta u$. Integrate by parts:

$$\begin{aligned} \tfrac{d^2H}{dt^2}(t) &= \textstyle\sum_{i,j=1}^n \int_U 2\frac{u_{x_i x_j}u_{x_i x_j}}{u} - 4\frac{u_{x_i}u_{x_j}u_{x_i x_j}}{u^2} \\ &\quad \textstyle +2|Du|^2\frac{\delta_{ij}u_{x_i}u_{x_j}}{u^3}dx \\ &\quad \textstyle -2\sum_{i,j=1}^n \int_{\partial U}\frac{u_{x_i}u_{x_i x_j}\nu^j}{u}dS. \end{aligned}$$

Then boundary term is

$$-\int_{\partial U} \frac{1}{u}\frac{\partial |Du|^2}{\partial \nu} dS \geq 0,$$

according to the Lemma. Consequently:

$$\begin{array}{rcl} \frac{d^2H(t)}{dt^2} & \geq & 2\int_U \frac{|D^2u|^2}{u} - 2\sum_{i,j=1}^n \frac{u_{x_i}u_{x_j}}{u^2}u_{x_ix_j} + \frac{|Du|^4}{u^3}dx \\ & \geq & 2\int_U \frac{|D^2u|^2}{u} - 2\frac{|Du|^2|D^2u|}{u^2} + \frac{|Du|^4}{u^3}dx \\ & \geq & 0, \end{array}$$

since

$$\begin{array}{rcl} \frac{|Du|^2|D^2u|}{u^2} & = & \left(\frac{|Du|^2}{u^{3/2}}\right)\left(\frac{|D^2u|}{u^{1/2}}\right) \\ & \leq & \frac{1}{2}\frac{|Du|^4}{u^3} + \frac{1}{2}\frac{|D^2u|^2}{u}. \end{array}$$

□

c. A differential form of Harnack's inequality

Again we consider positive solutions u of the heat equation

$$u_t - \Delta u = 0 \text{ in } U \times (0,\infty) \tag{27}$$

with

$$\frac{\partial u}{\partial \nu} = 0 \text{ on } \partial U \times [0,\infty). \tag{28}$$

We assume U is convex.

Lemma *We have*

$$\frac{u_t}{u} + \frac{n}{2t} \geq \frac{|Du|^2}{u^2}. \tag{29}$$

This estimate, derived in a different context by Li-Yau, is a time-dependent version of the pointwise estimate on γ from §A.2. Note that we can rewrite (29) to obtain the pointwise estimate

$$s_t + \frac{n}{2t} \geq \gamma$$

where as usual $s = \log u$ is the entropy density and $\gamma = \frac{|Du|^2}{u^2}$ is the local rate of entropy production.

Proof. 1. Write $v = \log u$; so that (27) becomes

$$v_t - \Delta v = |Dv|^2. \tag{30}$$

Set

$$w = \Delta v. \tag{31}$$

Then (30) implies

$$w_t - \Delta w = \Delta(|Dv|^2) = 2|D^2 v|^2 + 2Dv \cdot Dw. \tag{32}$$

But

$$w^2 = (\Delta v)^2 \leq n|D^2 v|^2,$$

and so (32) implies

$$w_t - \Delta w - 2Dv \cdot Dw \geq \frac{2}{n} w^2. \tag{33}$$

2. We will exploit the good term on the right hand side of (33). Set

$$\tilde{w} = tw + \frac{n}{2}. \tag{34}$$

Then

$$\begin{aligned} \tilde{w}_t - \Delta\tilde{w} - 2Dv \cdot D\tilde{w} &= w + t(w_t - \Delta w - 2Dv \cdot Dw) \\ &\geq w + \tfrac{2t}{n} w^2. \end{aligned} \tag{35}$$

Now (34) says

$$w = \frac{\tilde{w}}{t} - \frac{n}{2t}$$

and so

$$w^2 = \frac{\tilde{w}^2}{t^2} - \frac{n\tilde{w}}{t^2} + \frac{n^2}{4t^2}.$$

Thus (35) implies

$$\tilde{w}_t - \Delta\tilde{w} - 2Dv \cdot D\tilde{w} \geq -\frac{1}{t}\tilde{w}. \tag{36}$$

3. Now

$$\begin{aligned} \tfrac{\partial\tilde{w}}{\partial\nu} &= t\tfrac{\partial w}{\partial\nu} \\ &= t\tfrac{\partial}{\partial\nu}(v_t - |Dv|^2) \text{ on } \partial U \times [0,\infty) \end{aligned}$$

owing to (30), (31). Since $\frac{\partial v}{\partial\nu} = \frac{1}{u}\frac{\partial u}{\partial\nu} = 0$ on $\partial U \times [0,\infty)$,

$$\frac{\partial}{\partial\nu}(v_t) = \frac{\partial}{\partial t}\left(\frac{\partial v}{\partial\nu}\right) = 0 \text{ on } \partial U \times [0,\infty).$$

Also, the Lemma in §B gives

$$\frac{\partial}{\partial \nu}|Dv|^2 \leq 0 \text{ on } \partial U \times [0,\infty).$$

Thus

$$\frac{\partial \tilde{w}}{\partial \nu} \geq 0 \text{ on } \partial U \times [0,\infty). \tag{37}$$

4. Fix $\varepsilon > 0$ so small that

$$\tilde{w} = tw + \frac{n}{2} > 0 \text{ on } U \times \{t = \varepsilon\}. \tag{38}$$

Then (36)–(38) and the maximum principle for parabolic PDE imply

$$\tilde{w} \geq 0 \text{ in } U \times [\varepsilon, \infty).$$

This is true for all small $\varepsilon > 0$, and so

$$tw + \frac{n}{2} \geq 0 \text{ in } U \times (0,\infty).$$

But $w = \Delta v = v_t - |Dv|^2 = \frac{u_t}{u} - \frac{|Du|^2}{u^2}$. Estimate (33) follows. □

The following form of Harnack's inequality is a

Corollary. *For $x_1, x_2 \in \bar{U}$, $0 < t_1 < t_2$, we have*

$$u(x_1,t_1) \leq \left(\frac{t_2}{t_1}\right)^{n/2} e^{\frac{|x_2-x_1|^2}{4(t_2-t_1)}} u(x_2,t_2). \tag{39}$$

Proof. As before, take $v = \log u$. Then

(40)

$$\begin{aligned} v(x_2,t_2) - v(x_1,t_1) &= \int_0^1 \tfrac{d}{ds} v(sx_2 + (1-s)x_1, st_2 + (1-s)t_1) ds \\ &= \int_0^1 Dv \cdot (x_2 - x_1) + v_t(t_2 - t_1) ds \\ &\geq \int_0^1 -|Dv|\ |x_2 - x_1| + \left(|Dv|^2 - \tfrac{n}{2(st_2 + (1-s)t_1)}\right)(t_2 - t_1) ds \\ &\geq -\tfrac{n}{2} \log\left(\tfrac{t_2}{t_1}\right) - \tfrac{|x_2-x_1|^2}{4(t_2-t_1)}. \end{aligned}$$

Here we used the inequality $ab \leq \varepsilon a^2 + \frac{1}{4\varepsilon} b^2$ and the identity

$$\int_0^1 \frac{t_2 - t_1}{t_1 + s(t_2 - t_1)} ds = \log\left(\frac{t_2}{t_1}\right).$$

Exponentiate both sides of (40) to obtain (39). □

3. Clausius inequality

Day [D, Chapters 3,4] has noted that the heat equation (and related second-order parabolic PDE) admit various estimates which are reminiscent of the classical Clausius inequality from Chapter II. We recount in this section some simple cases of his calculations.

We hereafter assume $u > 0$ is a smooth solution of

$$u_t - \sum_{i,j=1}^{n} (a^{ij} u_{x_i})_{x_j} = 0 \text{ in } U \times (0, \infty) \tag{1}$$

subject now to the *prescribed temperature* condition

$$u(\cdot, t) = \tau(t) \text{ on } \partial U, \tag{2}$$

where $\tau : [0, \infty) \to (0, \infty)$ is a given, smooth function.

a. Cycles

Let us assume that $T > 0$ and τ is *T-periodic*:

$$\tau(t + T) = \tau(t) \text{ for all } t \geq 0. \tag{3}$$

We call a T-periodic solution of (1), (2) a *cycle*.

Lemma 1 *Corresponding to each T-periodic τ as above, there exists a unique cycle u.*

Proof. 1. Given a smooth function $g : \bar{U} \to (0, \infty)$, with $g = \tau(0)$ on ∂U, we denote by u the unique smooth solution of

$$\begin{cases} u_t - \sum_{i,j=1}^{\infty} (a^{ij} u_{x_i})_{x_j} = 0 & \text{in } U_T \\ u = \tau & \text{on } \partial U \times [0, T] \\ u = g & \text{on } U \times \{t = 0\}. \end{cases} \tag{4}$$

2. Let $\tilde{g}$ be another smooth function and define $\tilde{u}$ similarly. Then

$$\begin{aligned} \tfrac{d}{dt} \left(\textstyle\int_U (u - \tilde{u})^2 dx \right) &= 2 \textstyle\int_U (u_t - \tilde{u}_t)(u - \tilde{u}) dx \\ &= -2 \textstyle\int_U \sum_{i,j=1}^{n} a^{ij} (u_{x_i} - \tilde{u}_{x_i})(u_{x_j} - \tilde{u}_{x_j}) dx \\ &\leq -2\theta \textstyle\int_U |D(u - \tilde{u})|^2 dx, \end{aligned}$$

there being no boundary term when we integrate by parts, as $u - \tilde{u} = \tau - \tau = 0$ on ∂U. A version of *Poincaré's inequality* states

$$\int_U w^2 dx \leq C \int_U |Dw|^2 dx$$

for all smooth $w : \bar{U} \to \mathbb{R}$, with $w = 0$ on ∂U. Thus

$$\frac{d}{dt}\left(\int_U (u-\tilde{u})^2 dx\right) \leq -\mu \int_U (u-\tilde{u})^2 dx$$

for some $\mu > 0$ and all $0 \leq t \leq T$. Hence

$$\int_U (u(\cdot,T) - \tilde{u}(\cdot,T))^2 dx \leq e^{-\mu T} \int_U (g-\tilde{g})^2 dx. \tag{5}$$

Define $\Lambda(g) = u(\cdot,T)$, $\Lambda(\tilde{g}) = \tilde{u}(\cdot,T)$. As $e^{-\mu T/2} < 1$, Λ extends to a strict contraction from $L^2(U)$ into $L^2(U)$. Thus Λ has a unique fixed point $g \in L^2(U)$. Parabolic regularity theory implies g is smooth, and the corresponding smooth solution u of (4) is the cycle. □

b. Heating

Let u be the unique cycle corresponding to τ and recall from §A.1 that

$$\mathbf{q} = -ADu = \text{ heat flux.}$$

Thus

$$Q(t) = -\int_{\partial U} \mathbf{q} \cdot \boldsymbol{\nu} dS = \int_{\partial U} \frac{\partial u}{\partial \nu_A} dS \tag{6}$$

represents the *total heat flux into U* from its exterior at time $t \geq 0$. We define as well

$$\begin{cases} \tau^+ &= \sup\{\tau(t) \mid 0 \leq t \leq T,\ Q(t) > 0\} \\ \tau^- &= \inf\{\tau(t) \mid 0 \leq t \leq T,\ Q(t) < 0\} \end{cases} \tag{7}$$

to denote, respectively, the *maximum temperature at which heat is absorbed* and *minimum temperature at which heat is emitted*.

Theorem 1 (i) *We have*

$$\int_0^T \frac{Q}{\tau} dt \leq 0, \tag{8}$$

which strict inequality unless τ is constant.

(ii) *Furthermore if τ is not constant,*

$$\tau^- < \tau^+. \tag{9}$$

Notice that (8) is an obvious analogue of Clausius' inequality and (9) is a variant of classical estimates concerning the efficiency of cycles. In particular (9) implies that it is not

possible for heat to be absorbed only at temperatures below some given temperature τ_0 and to be emitted only at temperatures above τ_0. This is of course a form of the Second Law.

Proof. 1. Write $v = \log u$, so that

$$v_t - \sum_{i,j=1}^{n} (a^{ij} v_{x_i})_{x_j} = \sum_{i,j=1}^{n} a^{ij} v_{x_i} v_{x_j} = \gamma \geq 0.$$

Then

$$\begin{array}{rcl} \frac{d}{dt}\left(\int_U v(\cdot,t)dx\right) & = & \int_{\partial U} \frac{\partial v}{\partial \nu_A} dS + \int_U \gamma dx \\ & \geq & \int_{\partial U} \frac{1}{u} \frac{\partial u}{\partial \nu_A} dS \\ & = & \frac{Q(t)}{\tau(t)}, \end{array}$$

since $u(\cdot,t) = \tau(t)$ on ∂U. As $t \mapsto v(\cdot,t)$ is T-periodic, we deduce (8) upon integrating the above inequality for $0 \leq t \leq T$. We obtain as well a strict inequality in (8) unless

$$\int_0^T \int_U \gamma dx dt = 0,$$

which identity implies

$$\int_0^T \int_U |Dv|^2 dx dt = 0.$$

Thus $x \mapsto v(x,t)$ is constant for each $0 \leq t \leq T$ and so

$$u(x,t) \equiv \tau(t) \qquad (x \in U)$$

for each $0 \leq t \leq T$. But then the PDE (1) implies $u_t \equiv 0$ in U_T and so $t \mapsto \tau(t)$ is constant.

2. We now adapt a calculation from §II.A.3. If τ is not constant, then

$$\begin{array}{rcl} 0 > \int_0^T \frac{Q(t)}{\tau(t)} dt & = & \int_0^T \frac{Q^+(t) - Q^-(t)}{\tau(t)} dt \\ & \geq & \frac{1}{\tau^+} \int_0^T Q^+(t) dt - \frac{1}{\tau^-} \int_0^T Q^-(t) dt \\ & = & \frac{1}{\tau^+} \int_0^T \frac{|Q(t)| + Q(t)}{2} dt - \frac{1}{\tau^-} \int_0^T \frac{|Q(t)| - Q(t)}{2} dt \\ & = & \frac{1}{2}\left(\frac{1}{\tau^+} - \frac{1}{\tau^-}\right) \int_0^T |Q(t)| dt \\ & + & \frac{1}{2}\left(\frac{1}{\tau^+} + \frac{1}{\tau^-}\right) \int_0^T Q(t) dt. \end{array} \tag{10}$$

But the PDE (1) implies

$$\int_0^T Q(t) dt = \int_0^T \left(\frac{d}{dt} \int_U u(\cdot,t) dx\right) dt = 0,$$

since u is T-periodic. Hence (10) forces

$$\frac{1}{\tau^+} - \frac{1}{\tau^-} < 0.$$

□

See Day [D, p. 64] for an interesting estimate from below on $\tau^+ - \tau^-$.

c. Almost reversible cycles

Recall from Chapter II that the Clausius inequality becomes an equality for any reversible cycle. Furthermore the model discussed in §II.A.4 suggests that real, irreversible cycles approximate ideal, reversible cycles if the former are traversed very slowly. Following Day [D, Chapter 3], we establish next an analogue for our PDE (1).

Definition. We say a family of functions $\{\tau_\varepsilon\}_{0<\varepsilon\leq 1}$ is *slowly varying* if there exist times $\{T_\varepsilon\}_{0<\varepsilon\leq 1}$ and constants $0 < c \leq C$ so that

$$\text{(11)} \qquad \begin{cases} \text{(a)} & \tau_\varepsilon : [0,\infty) \to (0,\infty) \text{ is } T_\varepsilon\text{-periodic} \\ \text{(b)} & \tau_\varepsilon \geq c \\ \text{(c)} & T_\varepsilon \leq C/\varepsilon \\ \text{(d)} & |\dot{\tau}_\varepsilon| \leq C\varepsilon,\ |\ddot{\tau}_\varepsilon| \leq C\varepsilon^2 \end{cases}$$

for all $\varepsilon > 0$, $t \geq 0$.

For any τ_ε as above, let u_ε be the corresponding cycle, and set

$$Q_\varepsilon(t) = \int_{\partial U} \frac{\partial u_\varepsilon}{\partial \nu_A}(\cdot, t) dS.$$

Theorem 2 *We have*

$$\text{(12)} \qquad \int_0^{T_\varepsilon} \frac{Q_\varepsilon}{\tau_\varepsilon} dt = O(\varepsilon) \text{ as } \varepsilon \to 0.$$

Estimate (12) is a sort of approximation to the Clausius equality for reversible cycles.

Proof. 1. Let $w = w(x)$ be the unique smooth solution of

$$\text{(13)} \qquad \begin{cases} -\sum_{i,j=1}^n (a^{ij} w_{x_i})_{x_j} &= 1 \quad \text{in } U \\ w &= 0 \quad \text{on } \partial U, \end{cases}$$

and set

$$\text{(14)} \qquad \tilde{u}(x,t) := u_\varepsilon(x,t) - \tau_\varepsilon(t) + w(x)\dot{\tau}_\varepsilon(t)$$

for $x \in U$, $0 \le t \le T_\varepsilon$. Then (1), (13) imply

$$\left\{ \begin{array}{rcll} \tilde{u}_t - \sum_{i,j=1}^n (a^{ij}\tilde{u}_{x_i})_{x_j} & = & w(x)\ddot{\tau}_\varepsilon(t) & \text{in } U_{T_\varepsilon} \\ \tilde{u} & = & 0 & \text{on } \partial U \times [0, T_\varepsilon]. \end{array} \right. \tag{15}$$

Now

$$\begin{array}{rcl} Q_\varepsilon(t) & = & \int_{\partial U} \frac{\partial u_\varepsilon}{\partial \nu_A} dS = \frac{d}{dt}\int_U u_\varepsilon(\cdot,t)dx \\ & = & |U|\dot{\tau}_\varepsilon(t) - \left(\int_U w\ dx\right)\ddot{\tau}_\varepsilon(t) + R(t), \end{array} \tag{16}$$

for

$$R(t) = \int_U \tilde{u}_t(\cdot,t)dx. \tag{17}$$

2. We now assert that

$$\int_0^{T_\varepsilon} R^2(t)dt = O(\varepsilon^3) \text{ as } \varepsilon \to 0. \tag{18}$$

To verify this claim, multiply the PDE (15) by $\tilde{u}_t$ and integrate over U_{T_ε}:

$$\begin{array}{l} \int_0^{T_\varepsilon}\int_U \tilde{u}_t^2 dxdt + \int_0^{T_\varepsilon}\int_U \sum_{i,j=1}^n a^{ij}\tilde{u}_{x_i}\tilde{u}_{x_j t}dxdt \\ \quad = \int_0^{T_\varepsilon}\int_U w\ddot{\tau}_\varepsilon\tilde{u}_t dxdt. \end{array} \tag{19}$$

The second term on the left is

$$\int_0^{T_\varepsilon} \frac{d}{dt}\left(\frac{1}{2}\int_U \sum_{i,j=1}^n a^{ij}\tilde{u}_{x_i}\tilde{u}_{x_j}dx\right)dt = 0,$$

owing to the periodicity of $u_\varepsilon, \tau_\varepsilon$ and thus $\tilde{u}$. The expression on the right hand side of (19) is estimated by

$$\begin{array}{l} \frac{1}{2}\int_0^T\int_U \tilde{u}_t^2 dxdt + C\int_0^{T_\varepsilon} |\ddot{\tau}_\varepsilon|^2 dt \\ \quad \le \frac{1}{2}\int_0^T\int_U \tilde{u}_t^2 dxdt + O(\varepsilon^3), \end{array}$$

since $T_\varepsilon \le C/\varepsilon$, $|\ddot{\tau}_\varepsilon| \le C\varepsilon^2$. So (19) implies

$$\int_0^{T_\varepsilon}\int_U \tilde{u}_t^2 dxdt = O(\varepsilon^3),$$

and thus

$$\begin{array}{rcl} \int_0^{T_\varepsilon} R^2(t)dt & = & \int_0^{T_\varepsilon}\left(\int_U \tilde{u}_t dx\right)^2 dt \\ & \le & |U|\int_0^{T_\varepsilon}\int_U \tilde{u}_t^2 dxdt = O(\varepsilon^3). \end{array}$$

This proves (18).

3. Return now to (16). We have

$$\begin{aligned} \int_0^{T_\varepsilon} \frac{Q_\varepsilon}{\tau_\varepsilon} dt &= |U| \int_0^{T_\varepsilon} \frac{\dot{\tau}_\varepsilon}{\tau_\varepsilon} dt \\ &- \left(\int_U w dx\right) \int_0^{T_\varepsilon} \frac{\ddot{\tau}_\varepsilon}{\tau_\varepsilon} dt + \int_0^{T_\varepsilon} \frac{R}{\tau_\varepsilon} dt. \end{aligned} \tag{20}$$

The first term on the right is zero, since $\frac{\dot{\tau}_\varepsilon}{\tau_\varepsilon} = \frac{d}{dt}(\log \tau_\varepsilon)$ and τ_ε is T_ε-periodic. The second term is estimated by

$$C|T_\varepsilon| \sup |\ddot{\tau}_\varepsilon| = O(\varepsilon),$$

and the third term is less than or equal

$$\frac{T_\varepsilon^{1/2}}{c} \left(\int_0^{T_\varepsilon} R^2 dt\right)^{1/2} \leq \frac{C}{\varepsilon^{1/2}} \varepsilon^{3/2} = O(\varepsilon),$$

according to (18). This all establishes (12). □

Remark. Under the addition assumption that $|\dddot{\tau}_\varepsilon| \leq C\varepsilon^3$, Day proves:

$$\int_0^{T_\varepsilon} \frac{Q_\varepsilon}{\tau_\varepsilon} dt + A \int_0^{T_\varepsilon} \left(\frac{Q_\varepsilon}{\tau_\varepsilon}\right)^2 dt = O(\varepsilon^2)$$

where

$$A = \frac{1}{|U|^2} \int_U w dx.$$

See [D, p. 53–61]. □

CHAPTER 5: Conservation laws and kinetic equations

The previous chapter considered linear, second-order PDE which directly model heat conduction. This chapter by contrast investigates various nonlinear, first-order PDE, mostly in the form of conservation laws. The main theme is the use of entropy inspired concepts to understand *irreversibility in time*.

A. Some physical PDE

1. Compressible Euler equations

We recall here from §III.C the *compressible Euler's equations*

$$\left\{ \begin{array}{rcl} \frac{D\rho}{Dt} + \rho \text{ div } \mathbf{v} & = & 0 \\ \rho \frac{D\mathbf{v}}{Dt} & = & -Dp \end{array} \right. \tag{1}$$

where $\mathbf{v} = (v^1, v^2, v^3)$ is the velocity, ρ is the mass density, and p is the pressure.

a. Equation of state

Our derivation in Chapter III shows that p can be regarded as a function of s (the entropy density/unit mass) and v (the specific volume). Now if the fluid motion is *isentropic*, we can take s to be constant, and so regard p as a function only of v. But $v = \rho^{-1}$ and so we may equivalently take p as a function of ρ:

$$p = p(\rho). \tag{2}$$

This is an equation of state, the precise form of which depends upon the particular fluid we are investigating.

Assume further that the fluid is a *simple ideal gas*. Recall now formula (9) from §I.F, which states that at equilibrium

$$PV^\gamma = \text{ constant}, \tag{3}$$

where $\gamma = \frac{C_P}{C_V} > 1$.

Since we are assuming our flow is isentropic, it seems plausible to assume a local version of (3) holds:

$$pv^\gamma = \kappa, \tag{4}$$

κ denoting some positive constant. Thus for an isentropic flow of a simple ideal gas the general equation of state (2) reads

$$p = \kappa \rho^\gamma. \tag{5}$$

b. Conservation law form

For later reference, we recast Euler's equations (1). To do so, let us note that the second equation in (1) says

$$\rho\left(v_t^i + \sum_{j=1}^{3} v^j v_{x_j}^i\right) = -p_{x_i} \qquad (i = 1, 2, 3).$$

Hence

$$\begin{aligned}(\rho v^i)_t &= \rho_t v^i + \rho v_t^i \\ &= -v^i \textstyle\sum_{j=1}^3 (\rho v^j)_{x_j} - \rho \sum_{j=1}^3 v^j v_{x_j}^i - p_{x_i}, \\ &= -\textstyle\sum_{j=1}^3 (\rho v^i v^j)_{x_j} - p_{x_i} \qquad (i = 1, 2, 3).\end{aligned}$$

Therefore we can rewrite Euler's equations (1) to read

$$\text{(6)} \qquad \begin{cases} \rho_t + \ \operatorname{div}(\rho \mathbf{v}) &= 0 \\ (\rho \mathbf{v})_t + \ \operatorname{div}(\rho \mathbf{v} \otimes \mathbf{v} + pI) &= 0 \end{cases}$$

where $\mathbf{v} \otimes \mathbf{v} = ((v^i v^j))$ and $p = p(\rho)$. This is the *conservation law form* of the equations, expressing conservation of mass and linear momentum.

2. Boltzmann's equation

Euler's equations (1), (6) are PDE describing the *macroscopic* behavior of a fluid in terms of $\mathbf{v}$ and ρ. On the other hand the *microscopic* behavior is presumably dictated by the dynamics of a huge number ($\approx N_A \approx 6.02 \times 10^{23}$) of interacting particles. The key point is this: of the really large number of coordinates needed to characterize the details of particle motion, only a very few parameters persist at the macroscopic level, after "averaging over the microscopic dynamics". Understanding this transition from small to large scale dynamics is a fundamental problem in mathematical physics.

One important idea is to study as well the *mesoscopic* behavior, which we can think of as describing the fluid behavior at middle-sized scales. The relevant PDE here are generically called *kinetic equations*, the most famous of which is *Boltzmann's equation*.

a. A model for dilute gases

The unknown in Boltzmann's equation is a function

$$f : \mathbb{R}^3 \times \mathbb{R}^3 \times [0, \infty) \to [0, \infty),$$

such that

$$\begin{cases} f(x, v, t) \text{ is the density of the number of particles} \\ \text{at time } t \geq 0 \text{ and position } x \in \mathbb{R}^3, \text{ with} \\ \text{velocity } v \in \mathbb{R}^3. \end{cases}$$

Assume first that the particles do not interact. Then for each velocity $v \in \mathbb{R}^3$

$$\frac{d}{dt}\left(\int_{V(t)} f(x,v,t)dx\right) = 0,$$

where $V(t) = V + tv$ is the region occupied at time t by those particles initially lying within V and possessing velocity v. As §III.A, we deduce

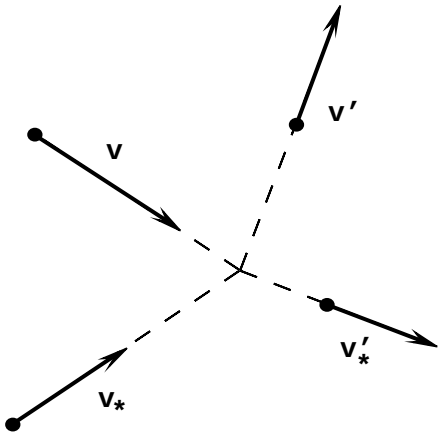
$$0 = \int_{V(t)} f_t + \text{ div}_x(fv)dx = \int_{V(t)} f_t + v \cdot D_x f dx.$$

Consequently

$$f_t + v \cdot D_x f = 0 \text{ in } \mathbb{R}^3 \times \mathbb{R}^3 \times (0,\infty) \tag{7}$$

if the particles do not interact.

Suppose now interactions do occur in the form of collisions, which we model as follows. Assume two particles, with velocities v and v_*, collide and after the collision have velocities v' and v'_*



We assume the particles all have the same mass m, so that conservation of momentum and kinetic energy dictate:

$$\begin{cases} \text{(a)} & v + v_* = v' + v'_* \\ \text{(b)} & |v|^2 + |v_*|^2 = |v'|^2 + |v'_*|^2, \end{cases} \tag{8}$$

where $v, v_*, v', v'_* \in \mathbb{R}^3$.

We now change variables, by writing

$$v' - v = -\alpha w$$

for $w \in S^2$ (= unit sphere in $\mathbb{R}^3$) and $\alpha = |v' - v| \geq 0$. Then (8)(a) implies

$$v'_* - v_* = \alpha w.$$

Furthermore

$$\begin{aligned} |v'|^2 + |v'_*|^2 &= |v - \alpha w|^2 + |v_* + \alpha w|^2 \\ &= |v|^2 - 2\alpha v \cdot w + \alpha^2 + |v_*|^2 + 2\alpha v_* \cdot w + \alpha^2. \end{aligned}$$

Consequently (8)(b) yields the identity:

$$\alpha = (v - v_*) \cdot w.$$

Hence

$$\left\{ \begin{aligned} v' &= v - [(v - v_*) \cdot w]w \\ v'_* &= v_* + [(v - v_*) \cdot w]w. \end{aligned} \right. \tag{9}$$

We next introduce the quadratic *collision operator*

$$\begin{aligned} Q(f,f)(v,\cdot) &= \int_{S^2} \int_{\mathbb{R}^3} [f(v',\cdot)f(v'_*,\cdot) - f(v,\cdot)f(v_*,\cdot)] \\ &\qquad B(v - v_*, w) dv_* dS(w) \end{aligned} \tag{10}$$

where dS means surface measure over S^2, v', v'_* are defined in terms of v, v_*, w by (9), and

$$B : \mathbb{R}^3 \times S^2 \to (0, \infty)$$

is given. We assume also that $B(z,w)$ in fact depends only on $|z|, |z \cdot w|$, this ensuring that model is rotationally invariant.

Boltzmann's equation is the integro/differential equation

$$f_t + v \cdot D_x f = Q(f,f) \text{ in } \mathbb{R}^3 \times \mathbb{R}^3 \times (0, \infty), \tag{11}$$

which differs from (7) with the addition of the collision operator $Q(f,f)$ on the right hand side. This term models the decrease in $f(v,x,t)$ and $f(v_*,x,t)$ and the gain in $f(v',x,t)$ and $f(v'_*,x,t)$, owing to collisions of the type illustrated above. The term B models the rate of collisions which start with velocity pairs v, v_* and result in velocity pairs v', v'_* given by (9). See Huang [HU, Chapter 3] for the physical derivation of (11).

b. H-Theorem

We henceforth assume f is a smooth solution of (11), with $f \geq 0$. We suppose as well that $f \to 0$ as $|x|, |v| \to \infty$, fast enough to justify the following calculations. Define then Boltzmann's *H-function*

$$H(t) = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} f \log f dv dx \qquad (t \geq 0), \tag{12}$$

concerning the form of which we will comment later.

Theorem 1 *We have*

$$\frac{dH}{dt} \leq 0 \quad \text{on } [0,\infty). \tag{13}$$

Proof. 1. Let us as shorthand notation hereafter write

$$f' = f(v',\cdot),\ f_* = f(v_*,\cdot),\ f'_* = f(v'_*,\cdot).$$

Thus

$$Q(f,f) = \int_{S^2}\int_{\mathbb{R}^3}[f'f'_* - ff_*]B(v-v_*,w)dv_*dS.$$

2. We now *claim* that if $\psi : \mathbb{R}^3 \to \mathbb{R}$ is smooth, $\psi = \psi(v)$, then

$$\int_{\mathbb{R}^3}\psi(v)Q(f,f)(v)dv = \frac{1}{4}\int_{S^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}(f'f'_* - ff_*)(\psi+\psi_*-\psi'-\psi'_*)Bdvdv_*dS. \tag{14}$$

This identity is valid since

1. interchanging v with v_* does not change the integrand on the left hand side of (14),
2. interchanging (v,v_*) with (v',v'_*) changes the sign of the integrand, and
3. interchanging (v,v_*) with (v'_*,v') changes the sign as well.

More precisely, write B_1 to denote the left hand side of (14). Then

$$\begin{array}{rcl} B_2 & := & \int_{S^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\psi_*(f'f'_* - ff_*)B(v-v_*,w)dvdv_*dS \\ & = & \int_{S^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\psi(f'_*f' - f_*f)B(v_*-v,w)dv_*dvdS, \end{array}$$

where we relabeled variables by interchanging v and v_*. Since $B(z,w)$ depends only on $|z|$, $|z\cdot w|$, we deduce

$$B_2 = B_1.$$

Next set

$$B_3 := \int_{S^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\psi'(f'f'_* - ff_*)B(v-v_*,w)dvdv_*dS.$$

For each fixed $w \in S^2$, we change variables in $\mathbb{R}^3\times\mathbb{R}^3$ by mapping (v,v_*) to (v',v'_*), using the formulas (9). Then

$$\frac{\partial(v',v'_*)}{\partial(v,v_*)} = \begin{pmatrix} I-w\otimes w & w\otimes w \\ w\otimes w & I-w\otimes w \end{pmatrix}_{6\times 6},$$

and so

$$\left|\frac{\partial(v', v'_*)}{\partial(v, v_*)}\right| = 1.$$

Consequently

$$B_3 = \int_{S^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \psi'(f'f'_* - ff_*)B(v - v_*, w)dv'dv'_*dS.$$

The integrand is

$$\psi(v')(f(v', \cdot)f(v'_*, \cdot) - f(v_*, \cdot)f(v, \cdot))B(v - v_*, w)$$

and we can now regard v, v_* as functions of v', v'_*:

$$\left\{\begin{array}{rcl} v &=& v' - [(v' - v'_*) \cdot w]w \\ v_* &=& v'_* + [(v' - v'_*) \cdot w]w. \end{array}\right.$$

Next we simply *relabel* the variables above, and so write "v, v_*" for "v', v'_*", and vice-versa:

$$B_3 = \int_{S^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \psi(ff_* - f'f'_*)B(v' - v'_*, w)dvdv_*dS.$$

Now (9) implies

$$\left\{\begin{array}{rcl} |v - v_*| &=& |v' - v'_*| \\ (v - v_*) \cdot w &=& -(v' - v'_*) \cdot w; \end{array}\right.$$

and so, since $B(z, w)$ depends only on $|z|, |z \cdot w|$, we deduce

$$B_3 = -B_1.$$

Similarly we have

$$B_4 = -B_1,$$

for

$$B_4 := \int_{S^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \psi'_*(f'f'_* - ff_*)B(v - v_*, w)dvdv_*dS.$$

Combining everything, we discover

$$4B_1 = B_1 + B_2 - B_3 - B_4,$$

and this is the identity (14).

3. Now set $\psi(v) = \log f(v, \cdot)$ in (14). Then

(15)

$$\begin{array}{rcl} \int_{\mathbb{R}^3} \log f(v, \cdot)Q(f, f)(v, \cdot)dv &=& \frac{1}{4}\int_{S^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}(f'f'_* - ff_*)[\log(ff_*) - \log(f'f'_*)]Bdvdv_*dS \\ &\leq& 0, \end{array}$$

since $B \geq 0$ and log is increasing. Also put $\psi \equiv 1$, to conclude

$$\int_{\mathbb{R}^3} Q(f,f)(v,\cdot)dv = 0. \tag{16}$$

4. Thus

$$\begin{aligned} \tfrac{d}{dt}H(t) &= \textstyle\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} f_t(\log f + 1)dvdx \\ &= \textstyle\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}[-v\cdot D_x f + Q(f,f)](\log f + 1)dvdx \\ &\leq -\textstyle\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} v\cdot D_x f(\log f+1)dvdx \text{ by (15), (16)} \\ &= -\textstyle\int_{\mathbb{R}^3} v\cdot\left(\int_{\mathbb{R}^3} D_x(f\log f)dx\right)dv \\ &= 0. \end{aligned}$$

□

Remark. A smooth function $f : \mathbb{R}^3 \to [0,\infty)$, $f = f(v)$, is called a *Maxwellian* if

$$Q(f,f) \equiv 0 \text{ on } \mathbb{R}^3. \tag{17}$$

It is known that each Maxwellian has the form:

$$f(v) = ae^{-b|v-c|^2} \qquad (v \in \mathbb{R}^3) \tag{18}$$

for constants $a, b \in \mathbb{R}$, $c \in \mathbb{R}^3$: see Truesdell–Muncaster [T-M].

According to the proof of Theorem 1, we have

$$\frac{d}{dt}H(t) < 0$$

unless $v \mapsto f(x,v,t)$ is a Maxwellian for all $x \in \mathbb{R}^3$. This observation suggests that as $t \to \infty$ solutions of Boltzmann's equations will approach Maxwellians, that is

$$f(x,v,t) \approx a(x,t)e^{-b(x,t)|v-\mathbf{c}(x,t)|^2} \qquad (x,v \in \mathbb{R}^3) \tag{19}$$

for $t \gg 1$. □

c. H and entropy

We provide in this section some physical arguments suggesting *a connection between the H-function and entropy*. The starting point is to replace (19) by the equality

$$f(x,v,t) = a(x,t)e^{-b(x,t)|v-\mathbf{c}(x,t)|^2} \qquad (x,v \in \mathbb{R}^3,\ t \geq 0), \tag{20}$$

where $a, b : \mathbb{R}^3 \times [0,\infty) \to (0,\infty)$, $\mathbf{c} : \mathbb{R}^3 \times [0,\infty) \to \mathbb{R}^3$. In other words we are assuming that at each point x in space and instant t in time, the distribution $v \mapsto f(x,v,t)$ is a Maxwellian

and is thus determined by the macroscopic parameters $a = a(x,t)$, $b = b(x,t)$, $\mathbf{c} = \mathbf{c}(x,t)$. We intend to interpret these physically.

(i) It is first of all convenient to rewrite (20):

$$f(x,v,t) = \frac{n}{(2\pi\lambda)^{3/2}} e^{-\frac{|v-\mathbf{v}|^2}{2\lambda}}, \tag{21}$$

where $n, \lambda, \mathbf{v}$ are functions of (x,t), $n, \lambda > 0$. Then

$$\begin{cases} \text{(a)} & \int_{\mathbb{R}^3} f dv = n \\ \text{(b)} & \int_{\mathbb{R}^3} v f dv = n\mathbf{v} \\ \text{(c)} & \int_{\mathbb{R}^3} |v-\mathbf{v}|^2 f dv = 3n\lambda. \end{cases} \tag{22}$$

Thus (22)(a) says:

$$\int_{\mathbb{R}^3} f(x,v,t) dv = n(x,t), \tag{23}$$

where $n(x,t)$ is the *particle density* at $x \in \mathbb{R}^3$, $t \geq 0$. Introduce also

$$m = \text{ mass/particle.}$$

Then

$$\int_{\mathbb{R}^3} m f(x,v,t) dv = mn(x,t) =: \rho(x,t), \tag{24}$$

for $\rho(x,t)$ the *mass density*. Then (22)(b) implies

$$\int_{\mathbb{R}^3} mv f(x,v,t) dv = \rho(x,t)\mathbf{v}(x,t), \tag{25}$$

and thus $\mathbf{v}(x,t)$ is the macroscopic *velocity*. Using (22)(c) we deduce:

$$\int_{\mathbb{R}^3} \frac{m}{2}|v|^2 f(x,v,t) dv = \frac{1}{2}\rho(x,t)|\mathbf{v}(x,t)|^2 + \frac{3}{2}\rho(x,t)\lambda(x,t). \tag{26}$$

The term on the left is the total energy at (x,t) (since $\frac{m}{2}|v|^2$ is the kinetic energy of a particle with mass m and velocity v, and $f(x,v,t)$ is the number of such particles at (x,t)). The expression $\frac{1}{2}\rho|\mathbf{v}|^2$ on the right is the macroscopic kinetic energy. Thus the term $\frac{3}{2}\rho\lambda$ must somehow model macroscopic internal energy.

(ii) To further the interpretation we now suppose that our gas can be understood macroscopically as a *simple ideal gas*, as earlier discussed in §I.F. From that section we recall the equilibrium entropy function

$$S = R\log V + C_V \log T + S_0, \tag{27}$$

valid for mole number $N = 1$. Here

$$\begin{cases} S &= \text{entropy/mole} \\ C_V &= \text{heat capacity/mole.} \end{cases}$$

Now a mole of any substance contains Avagadro's number N_A of molecules: see Appendix A. Thus the mass of a mole of our gas is $N_A m$. Define now

$$\begin{cases} s &= \text{entropy/unit mass} \\ c_v &= \text{heat capacity/unit mass.} \end{cases}$$

Then

$$\begin{cases} s &= S/N_A m \\ c_v &= C_V/N_A m. \end{cases} \tag{28}$$

Recall also from §I.F that

$$\gamma = \frac{C_P}{C_V} > 1,\ C_P - C_V = R. \tag{29}$$

Then (27)–(29) imply:

$$\begin{aligned} s &= \tfrac{R\log V + C_V \log T}{N_A m} + s_0 \\ &= \tfrac{R}{N_A}\tfrac{(\log V + (\gamma-1)^{-1}\log T)}{m} + s_0 \\ &= \tfrac{k}{m}(\log V + (\gamma-1)^{-1}\log T) + s_0, \end{aligned} \tag{30}$$

where

$$k = \frac{R}{N_A} \tag{31}$$

is *Boltzmann's constant*. We now further hypothesize (as in Chapter III) that formula (30) makes sense at each point $x \in \mathbb{R}^3$, $t \geq 0$ for our nonequilibrium gas. That is, in (30) we replace

$$\begin{cases} s \text{ by } s(x,t) = \text{ entropy density/unit mass} \\ T \text{ by } \theta(x,t) = \text{ local temperature} \\ V \text{ by } \frac{1}{\rho(x,t)} = \text{ volume/unit mass.} \end{cases} \tag{32}$$

Inserting (32) into (30) gives:

$$s = \frac{k}{m}((\gamma-1)^{-1}\log\theta - \log\rho) + s_0. \tag{33}$$

(iii) Return now to (21). We compute for $x \in \mathbb{R}^3$, $t \geq 0$:

$$\begin{aligned} h(x,t) &:= \int_{\mathbb{R}^3} f(x,v,t) \log f(x,v,t) dv \\ &= \frac{n}{(2\pi\lambda)^{3/2}} \int_{\mathbb{R}^3} e^{-\frac{|v-\mathbf{v}|^2}{2\lambda}} \left[\log n - \frac{3}{2} \log(2\pi\lambda) - \frac{|v-\mathbf{v}|^2}{2\lambda} \right] dv \\ &= n \left(\log n - \frac{3}{2} \log \lambda + r_0 \right), \end{aligned}$$

r_0 denoting a constant. Since $nm = \rho$, we can rewrite:

$$h(x,t) = \frac{\rho}{m} \left(\log \rho - \frac{3}{2} \log \lambda + r_0 \right), \tag{34}$$

r_0 now a different constant.

Comparing now (33), (34), we deduce that up to arbitrary constants

$$\rho(x,t) s(x,t) = -k h(x,t) \qquad (x \in \mathbb{R}^3,\ t \geq 0), \tag{35}$$

provided λ is proportional to θ,

$$\lambda(x,t) = \kappa \theta(x,t) \qquad (\kappa > 0), \tag{36}$$

and $(\gamma - 1)^{-1} = 3/2$, that is

$$\gamma = \frac{5}{3}. \tag{37}$$

Making these further assumptions, we compute using (35) that

$$\begin{aligned} S(t) &:= \int_{\mathbb{R}^3} s(\cdot,t) dm = \int_{\mathbb{R}^3} s(\cdot,t) \rho(\cdot,t) dx \\ &= -k \int_{\mathbb{R}^3} h(\cdot,t) dx = -kH(t). \end{aligned}$$

Hence

$$S(t) = -kH(t) \qquad (t \geq 0). \tag{38}$$

So the total entropy at time t is just $-kH$ at time t and consequently *the estimate* (13) *that* $dH/dt \leq 0$ *is yet another version of Clausius' inequality.*

(iv) It remains to compute κ. Owing to (26), we expect

$$\frac{3}{2} \rho \lambda = \frac{3}{2} \rho \kappa \theta$$

to represent the total internal energy at (x,t). That is, $\frac{3}{2}\kappa\theta$ should be the internal energy/unit mass.

Now we saw in §I.F that the internal energy/mole at equilibrium is $C_V T$. Thus we can expect

$$\frac{3}{2}\kappa\theta = c_v\theta, \tag{39}$$

where we recall c_v is the heat capacity/unit mass. Thus (28), (39) imply:

$$\kappa = \frac{2}{3}\frac{C_V}{N_A m}.$$

But (29), (37) imply $C_V = \frac{3}{2}R$ and so

$$\kappa = \frac{R}{N_A m} = \frac{k}{m}. \tag{40}$$

We summarize by returning to (21):

$$f(x,v,t) = n\left(\frac{m}{2\pi k\theta}\right)^{3/2} e^{-\frac{m|v-\mathbf{v}|^2}{2k\theta}}, \tag{41}$$

where

$$\begin{aligned} n(x,t) &= \text{particle density at } (x,t) \\ \theta(x,t) &= \text{local temperature at } (x,t) \\ \mathbf{v}(x,t) &= \text{macroscopic fluid velocity at } (x,t). \end{aligned}$$

This formula is the *Maxwell–Boltzmann distribution* for v.

Remark. For reference later in Chapter VII, we rewrite (41) as

$$f = n\frac{e^{-\beta H}}{Z}, \tag{42}$$

for

$$\left\{ \begin{array}{rcl} \beta &=& \frac{1}{k\theta}, \\ H &=& \frac{m}{2}|v-\mathbf{v}|^2, \\ Z &=& \left(\frac{2\pi k\theta}{m}\right)^{3/2} = \int_{\mathbb{R}^3} e^{-\beta H} dv. \end{array} \right. \tag{43}$$

□

B. Single conservation law

Euler's and Boltzmann's equations are among the most important physical PDE but, unfortunately, there is no fully satisfactory mathematical theory available concerning the

existence, uniqueness and regularity of solutions for either. Much effort has focused therefore on certain simpler model PDE, the rigorous analysis of which presumably provides clues about the structure of solutions of Euler's and Boltzmann's PDE.

In this section we discuss a type of nonlinear first-order PDE called a *conservation law* and describe how entropy-like notions are employed to record irreversibility phenomena and in fact to define appropriate weak solutions. Following Lions, Perthame, Tadmor [L-P-T1] we introduce also a *kinetic approximation*, which is a sort of simpler analogue of Boltzmann's equation. In §C following we discuss *systems* of conservation laws.

1. Integral solutions

A PDE of the form

$$u_t + \text{ div } \mathbf{F}(u) = 0 \text{ in } \mathbb{R}^n \times (0,\infty) \tag{1}$$

is called a scalar *conservation law*. Here the unknown is

$$u : \mathbb{R}^n \times [0,\infty) \to \mathbb{R}$$

and we are given the *flux function*

$$\mathbf{F} : \mathbb{R} \to \mathbb{R}^n, \ \mathbf{F} = (F^1, \dots, F^n).$$

Physical interpretation. We regard $u = u(x,t)$ $(x \in \mathbb{R}^n, \ t \geq 0)$ as the density of some scalar conserved quantity. If V represents a fixed subregion of $\mathbb{R}^n$, then

$$\frac{d}{dt}\left(\int_V u(\cdot,t)dx\right) \tag{2}$$

represents the rate of change of the total amount of the quantity within V, and we assume this change equals the flux inward through ∂V:

$$-\int_{\partial V} \mathbf{F} \cdot \boldsymbol{\nu} dS. \tag{3}$$

We hypothesize that $\mathbf{F}$ is a function of u. Equating (2), (3) for any region V yields the conservation law (1). Note that (1) is a caricature of Euler's equations (6) in §A. □

Notation. We will sometimes rewrite (1) into *nondivergence form*

$$u_t + \mathbf{b}(u) \cdot Du = 0 \quad \text{ in } \mathbb{R}^n \times (0,\infty), \tag{4}$$

where

$$\mathbf{b} = \mathbf{F}', \ \mathbf{b} = (b^1, \dots, b^n). \tag{5}$$

We can interpret (4) as a *nonlinear transport equation*, for which the *velocity* $\mathbf{v} = \mathbf{b}(u)$ depends on the unknown density u. The left hand side of (4) is thus a sort of nonlinear variant of the material derivative $\frac{Du}{Dt}$ from Chapter III. The *characteristics* of (1) are solutions $x(\cdot)$ of the ODE

$$\dot{x}(t) = \mathbf{v}(x(t), t) = \mathbf{b}(u(x(t), t)) \qquad (t \geq 0). \tag{6}$$

□

We will study the *initial value problem*

$$\begin{cases} u_t + \text{ div } \mathbf{F}(u) &= 0 \text{ in } \mathbb{R}^n \times (0, \infty) \\ u &= g \text{ on } \mathbb{R}^n \times \{t = 0\}, \end{cases} \tag{7}$$

where $g \in L^1_{\text{loc}}(\mathbb{R}^n)$ is the initial density. The first difficulty in this subject is to understand the right way to interpret a function u as solving (7).

Definition. We say $u \in L^1_{\text{loc}}(\mathbb{R}^n \times (0, \infty))$ is an *integral solution* of (7) provided:

$$\int_0^\infty \int_{\mathbb{R}^n} uv_t + \mathbf{F}(u) \cdot Dv dx dt + \int_{\mathbb{R}^n} gv(\cdot, 0) dx = 0 \tag{8}$$

for all $v \in C_c^1(\mathbb{R}^n \times [0, \infty))$.

Examples.

(a) If

$$g(x) = \begin{cases} 1 & x < 0 \\ 0 & x > 0, \end{cases}$$

then

$$u(x, t) = \begin{cases} 1 & x < \frac{t}{2} \\ 0 & x > \frac{t}{2} \end{cases}$$

is an integral solution of

$$\begin{cases} u_t + \left(\frac{u^2}{2}\right)_x &= 0 \text{ in } \mathbb{R} \times (0, \infty) \\ u &= g \text{ on } \mathbb{R} \times \{t = 0\}. \end{cases} \tag{9}$$

(b) If, instead,

$$g(x) = \begin{cases} 0 & x < 0 \\ 1 & x > 0, \end{cases}$$

then

$$u_1(x,t) = \begin{cases} 0 & x < \frac{t}{2} \\ 1 & x > \frac{t}{2} \end{cases}$$

and

$$u_2(x,t) = \begin{cases} 0 & x < 0 \\ \frac{x}{t} & 0 < x < t \\ 1 & x > t \end{cases}$$

are both integral solutions of (9).

As explained in Smoller [S], [E1, Chapter III], etc., "the physically correct" integral solution of (b) is u_2. The function u from Example (a) admits a "physical shock", with which the characteristics collide. The function u_1 from Example (b) is wrong since it has a "nonphysical shock", from which characteristics emanate.

(c) If

$$g(x) = \begin{cases} 1 & x < 0 \\ 1 - x & 0 < x < 1 \\ 0 & x > 1, \end{cases}$$

then

$$\begin{aligned} u(x,t) &= \begin{cases} 1 & x \le t,\ 0 \le t \le 1 \\ \frac{1-x}{1-t} & t \le x \le 1,\ 0 \le t \le 1 \\ 0 & x \ge 1,\ 0 \le t \le 1 \end{cases} \\ &= \begin{cases} 1 & x < \frac{1+t}{2},\ t \ge 1 \\ 0 & x > \frac{1+t}{2},\ t \ge 1 \end{cases} \end{aligned}$$

is an integral solution of (9).

The function u is the physically correct solution of (9). Note carefully that although $g = u(\cdot, 0)$ is continuous, $u(\cdot, t)$ is discontinuous for times $t > 1$. Note also that this example illustrates *irreversibility*. If

$$\hat{g}(x) = \begin{cases} 1 & x \le \frac{1}{2} \\ 0 & x > \frac{1}{2}, \end{cases}$$

then the corresponding physically correct solution is

$$\hat{u}(x,t) = \begin{cases} 1 & x < \frac{1+t}{2} \\ 0 & x > \frac{1+t}{2}. \end{cases}$$

But then $u \equiv \hat{u}$ for times $t \ge 1$. □

2. Entropy solutions

We next introduce some additional mathematical structure which will clarify what we mean above by a "physically correct" solution.

Definition. We call $(\Phi, \mathbf{\Psi})$ an *entropy/entropy flux* pair for the conservation law (1) provided

(i) $\Phi : \mathbb{R} \to \mathbb{R}$ is convex

and

(ii) $\mathbf{\Psi} : \mathbb{R} \to \mathbb{R}^n$, $\mathbf{\Psi} = (\Psi^1, \dots, \Psi^n)$

satisfies

$$\mathbf{\Psi}' = \mathbf{b}\Phi'. \tag{10}$$

Thus

$$\Psi^i(z) = \int_0^z b^i(v)\Phi'(v)dv \qquad (i = 1, \dots, n) \tag{11}$$

up to additive constants. □

Motivation. Notice that it is a C^1-solution of (1) in some region of $\mathbb{R}^n \times (0, \infty)$, then (10) implies

$$\Phi(u)_t + \text{ div } \mathbf{\Psi}(u) = 0$$

there. We interpret this equality to mean that there is no entropy production within such a region. On the other hand our examples illustrate that integral solutions can be discontinuous, and in particular Examples (a), (b) suggest certain sorts of discontinuities are physically acceptable, others not.

We intend to employ entropy/entropy flux pairs to provide an *inequality* criterion, a kind of analogue of the Clausius–Duhem inequality, for selecting the proper integral solution. The easiest way to motivate all this is to introduce the regularized PDE

$$u_t^\varepsilon + \text{ div } \mathbf{F}(u^\varepsilon) = \varepsilon \Delta u^\varepsilon \text{ in } \mathbb{R}^n \times (0, \infty), \tag{12}$$

where $\varepsilon > 0$. By analogy with the incompressible Navier–Stokes equations ((18) in §III.C) we can regard the term "$\varepsilon \Delta u^\varepsilon$" as modelling viscous effects, which presumably tend to smear out discontinuities. And indeed it is possible to prove under various technical hypotheses that (12) has a smooth solution u^ε, subject to initial condition $u^\varepsilon = g$ on $\mathbb{R}^n \times \{t = 0\}$.

Take a smooth entropy/entropy flux pair $\Phi, \mathbf{\Psi}$ and compute:

$$\begin{aligned}
\Phi(u^\varepsilon)_t + \text{ div } \mathbf{\Psi}(u^\varepsilon) &= \Phi'(u^\varepsilon)u_t^\varepsilon + \mathbf{\Psi}'(u^\varepsilon) \cdot Du^\varepsilon \\
&= \Phi'(u^\varepsilon)(-\mathbf{b}(u^\varepsilon) \cdot Du^\varepsilon + \varepsilon \Delta u^\varepsilon) + \mathbf{\Psi}'(u^\varepsilon) \cdot Du^\varepsilon \\
&= \varepsilon \Phi'(u^\varepsilon)\Delta u \text{ by (10)} \qquad (13) \\
&= \varepsilon \text{ div}(\Phi'(u^\varepsilon)Du^\varepsilon) - \varepsilon \Phi''(u^\varepsilon)|Du^\varepsilon|^2 \\
&\leq \varepsilon \text{ div}(\Phi'(u^\varepsilon)Du^\varepsilon),
\end{aligned}$$

the inequality holding since Φ is convex. Now take $v \in C_c^1\ (\mathbb{R}^n \times (0,\infty))$, $v \geq 0$. Then (13) implies

$$\begin{aligned} \int_0^\infty \int_{\mathbb{R}^n} \Phi(u^\varepsilon) v_t + \mathbf{\Psi}(u^\varepsilon) \cdot Dv dx dt &= -\int_0^\infty \int_{\mathbb{R}^n} v(\Phi(u^\varepsilon)_t + \ \mathrm{div}(\mathbf{\Psi}(u^\varepsilon)) dx dt \\ &\geq -\varepsilon \int_0^\infty \int_{\mathbb{R}^n} v\ \mathrm{div}(\Phi'(u^\varepsilon) Du^\varepsilon) dx dt \\ &= \varepsilon \int_0^\infty \int_{\mathbb{R}^n} \Phi'(u^\varepsilon) Dv \cdot Du^\varepsilon dx dt. \end{aligned}$$

Assume now that as $\varepsilon \to 0$,

$$u^\varepsilon \to u \text{ boundedly, a.e.,} \tag{14}$$

and further we have the estimate

$$\sup_\varepsilon \int_0^\infty \int_{\mathbb{R}^n} \varepsilon |Du^\varepsilon|^2 dx dt < \infty. \tag{15}$$

Then send $\varepsilon \to 0$ above

$$\int_0^\infty \int_{\mathbb{R}^n} \Phi(u) v_t + \mathbf{\Psi}(u) \cdot Dv dx dt \geq 0. \tag{16}$$

This inequality motivates the following

Definition. We say that $u \in C([0,\infty);\ L^1(\mathbb{R}^n))$ is an *entropy solution* of

$$\begin{cases} u_t + \ \mathrm{div}\ \mathbf{F}(u) &= 0 \text{ in } \mathbb{R}^n \times (0,\infty) \\ u &= g \text{ on } \mathbb{R}^n \times \{t=0\} \end{cases} \tag{17}$$

provided

$$\Phi(u)_t + \ \mathrm{div}\ \mathbf{\Psi}(u) \leq 0 \tag{18}$$

in the weak sense for each entropy/entropy flux pair (Φ, Ψ), and

$$u(\cdot, 0) = g. \tag{19}$$

Remarks. (i) The meaning of (18) is that the integral inequality (16) holds for all $v \in C_c^1(\mathbb{R}^n \times (0,\infty))$, $v \geq 0$.

(ii) We can regard (18) as a form of the Clausius–Duhem inequality, except *that the sign is reversed*. Note carefully: if Φ, Ψ is an entropy/entropy flux pair, then $s = -\Phi(u)$ acts like a physical entropy density. The customary mathematical and physical usages of the term entropy differ in sign.

(iii) Since we have seen that $\Phi(u)_t + \ \mathrm{div}\ \mathbf{\Psi}(u) = 0$ in any region where u is C^1, the possible inequalities in (18) must arise only where u is not C^1, e.g. along shocks. We motivated (18)

by the vanishing viscosity method of sending $\varepsilon \to 0$ in (12). This is somewhat related to the model thermodynamic system introduced in §II.A.4 where we added dissipation to an ideal dissipationless model. In that setting, the ideal model arises if conversely we send the dissipation terms $R_1, R_2 \to 0$. By contrast, for conservation laws if we obtain u as the limit (14) of solutions u^ε of the viscous approximations (12), then u "remembers" this vanishing viscosity process in the structure of its discontinuities.

For instance in examples (a)–(b) above, the physically correct shocks do arise as the limit $\varepsilon \to 0$, whereas the physically incorrect shock cannot. (To be consistent, we should redefine the g's and thus the u's for large $|x|$, so that $u \in L^1$.) □

The existence of an entropy solution of (17) follows via the vanishing viscosity process, and the really important assertion is this theorem of Kruzkov:

Theorem *Assume that $u, \hat{u}$ are entropy solutions of*

$$\text{(20)} \qquad \begin{cases} u_t + \text{ div } \mathbf{F}(u) &= 0 \text{ in } \mathbb{R}^n \times (0,\infty) \\ u &= g \text{ on } \mathbb{R}^n \times \{t=0\} \end{cases}$$

and

$$\text{(21)} \qquad \begin{cases} \hat{u}_t + \text{ div } \mathbf{F}(\hat{u}) &= 0 \text{ in } \mathbb{R}^n \times (0,\infty) \\ \hat{u} &= \hat{g} \text{ on } \mathbb{R}^n \times \{t=0\}. \end{cases}$$

Then

$$\text{(22)} \qquad \|u(\cdot,t) - \hat{u}(\cdot,t)\|_{L^1(\mathbb{R}^n)} \le \|u(\cdot,s) - \hat{u}(\cdot,s)\|_{L^1(\mathbb{R}^n)}$$

for each $0 \le s \le t$.

In particular an *entropy solution of the initial value problem* (20) *is unique.*

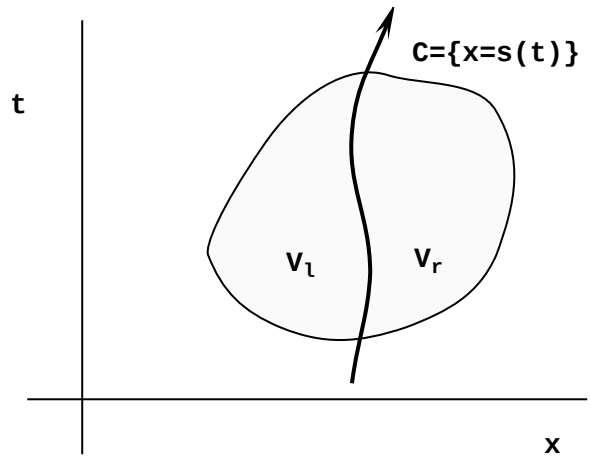
See for instance [E1, §11.4.3] for proof.

3. Condition E

We illustrate the meaning of the entropy condition for $n = 1$ by examining more closely the case that u is a piecewise smooth solution of

$$\text{(23)} \qquad u_t + F(u)_x = 0 \text{ in } \mathbb{R} \times (0,\infty).$$

More precisely assume that some region $V \subset \mathbb{R} \times (0,\infty)$ is subdivided into a left region V_l and a right region V_r by a smooth curve C, parametrized by $\{x = s(t)\}$:



Assume that u is smooth in both $\bar{V_l}$ and $\bar{V_r}$, and further u satisfies the condition

$$\Phi(u)_t + \Psi(u)_x \leq 0 \text{ in } V \tag{24}$$

in the weak sense, for each entropy/entropy flux pair (Φ, Ψ). Thus

$$\iint_V \Phi(u)v_t + \Psi(u)v_x dxdt \geq 0 \tag{25}$$

for each $v \in C_0^1(V)$, with $v \geq 0$. Here

$$\begin{cases} \Phi : \mathbb{R} \to \mathbb{R} \text{ is convex, and} \\ \Psi' = b\Phi' \text{ for } b = F'. \end{cases} \tag{26}$$

First take $v \in C_c^1(V_l)$, $v \geq 0$. Then, since u is smooth in V_l, we can integrate by parts in (25) to deduce

$$\iint_{V_l} [\Phi(u)_t + \Psi(u)_x]v dxdt \leq 0.$$

This inequality is valid for each v as above, whence

$$\Phi(u)_t + \Psi(u)_x \leq 0 \text{ in } V_l.$$

Take $\Phi(z) = \pm z$, $\Psi(z) = \pm F(z)$, to conclude

$$u_t + F(u)_x = 0 \text{ in } V_l.$$

But then (26) implies

$$\Phi(u)_t + \Psi(u)_x = 0 \text{ in } V_l. \tag{27}$$

Similarly

$$u_t + F(u)_x = 0 \text{ in } V_r,$$

$$\Phi(u)_t + \Psi(u)_x = 0 \text{ in } V_r. \tag{28}$$

Next take $v \in C_c^1(V)$, $v \geq 0$. Then (25) says

$$\iint_{V_t} \Phi(u)v_t + \Psi(u)v_x dxdt + \iint_{V_r} \Phi(u)v_t + \Psi(u)v_x dxdt \geq 0.$$

Integrate by parts in each term, recalling (27), (28), to deduce

$$\int_C v[(\Phi(u_l) - \Phi(u_r))\nu^2 + (\Psi(u_l) - \Psi(u_r))\nu^1]dl \geq 0 \tag{29}$$

where $\boldsymbol{\nu} = (\nu^1, \nu^2)$ is the outer unit normal to V_l along C, u_l is the limit of u from the left along C, and u_r is the limit from the right. Since

$$\boldsymbol{\nu} = \frac{1}{(1 + (\dot{s})^2)^{1/2}}(1, -\dot{s})$$

and $v \geq 0$ is arbitrary, we conclude from (29) that

$$\dot{s}(\Phi(u_r) - \Phi(u_l)) \geq \Psi(u_r) - \Psi(u_l) \text{ along } C. \tag{30}$$

Taking $\Phi(z) = \pm z$, $\Psi(z) = \pm F(z)$, we obtain the *Rankine–Hugoniot* jump condition

$$\dot{s}(u_r - u_l) = F(u_r) - F(u_l). \tag{31}$$

Select now a time t, and suppose $u_l < u_r$. Fix $u_l < u < u_r$ and define the entropy/entropy flux pair

$$\begin{cases} \Phi(z) &= (z-u)^+ \\ \Psi(z) &= \int_{u_l}^z \operatorname{sgn}^+(v-u)F'(v)dv. \end{cases}$$

Then

$$\begin{cases} \Phi(u_r) - \Phi(u_l) &= u_r - u \\ \Psi(u_r) - \Psi(u_l) &= F(u_r) - F(u). \end{cases}$$

Consequently (30) implies

$$\dot{s}(u - u_r) \leq F(u) - F(u_r). \tag{32}$$

Combine (31), (32):

$$F(u) \geq \frac{F(u_r) - F(u_l)}{u_r - u_l}(u - u_r) + F(u_r) \qquad (u_l \leq u \leq u_r). \tag{33}$$

This inequality holds for each $u_l \le u \le u_r$ and says that the graph of F on the internal $[u_l, u_r]$ lies above the line segment connecting $(u_l, F(u_l))$ to $(u_r, F(u_r))$.

A similar proof shows that if $u_l > u_r$, then

$$F(u) \le \left[\frac{F(u_r) - F(u_l)}{u_r - u_l}\right](u - u_r) + F(u_r) \qquad (u_r \le u \le u_l) \tag{34}$$

The inequalities (33), (34) are called *Oleinik's condition E*.

Remarks. (i) In particular,

$$\begin{cases} \text{if } F \text{ is strictly convex, then } u_l \ge u_r \\ \text{and} \\ \text{if } F \text{ is strictly concave, then } u_l \le u_r. \end{cases}$$

□

(ii) If (33) or (34) holds, then

$$F'(u_r) \le \dot{s} = \frac{F(u_r) - F(u_l)}{u_r - u_l} \le F'(u_l).$$

As characteristics move with speed $b = F'$, we see that characteristics can only collide with the shock and cannot emanate from it. The same conclusion follows from (34). *This geometric observation records the irreversibility inherent in the entropy condition* (24).

□

4. Kinetic formulation

Our intention next is to introduce and study a sort of *kinetic formulation* of the conservation law $u_t + \text{ div } \mathbf{F}(u) = 0$. If we think of this PDE as a simplified version of Euler's equations, the corresponding kinetic PDE is then a rough analogue of Boltzmann's equation. The following is taken from Perthame–Tadmor [P-T] and Lions–Perthame–Tadmor [L-P-T1].

We will study the *kinetic equation*

$$w_t + \mathbf{b}(y) \cdot D_x w = m_y \text{ in } \mathbb{R}^n \times \mathbb{R} \times (0, \infty), \tag{35}$$

where

$$w : \mathbb{R}^n \times \mathbb{R} \times (0, \infty) \to \mathbb{R}, \ w = w(x, y, t),$$

is the unknown, $\mathbf{b} = \mathbf{F}'$ as in §2, and m is a nonnegative Radon measure on $\mathbb{R}^n \times \mathbb{R} \times (0, \infty)$. Hence

$$m_y = \frac{\partial}{\partial y} m.$$

We interpret w as solving (35) in the weak (i.e. distribution) sense.

We can think of y as a variable parameterizing the velocity field $\mathbf{v} = \mathbf{b}(y)$ and so—in analogy with Boltzmann's equation—interpret $w(x, y, t)$ as the density of particles with velocity $\mathbf{v} = \mathbf{b}(y)$ at the point $x \in \mathbb{R}^n$ and time $t \geq 0$. Then

$$u(x,t) := \int_{\mathbb{R}} w(x,y,t)dy \tag{36}$$

should represent the density at (x, t). The idea will be to show under certain circumstances that u solves the conservation law $u_t + \text{ div } \mathbf{F}(u) = 0$.

To facilitate this interpretation, we introduce the *pseudo-Maxwellian*

$$\chi_a(y) = \begin{cases} 1 & \text{if } 0 < y \leq a \\ -1 & \text{if } a \leq y \leq 0 \\ 0 & \text{otherwise.} \end{cases} \tag{37}$$

for each parameter $a \in \mathbb{R}$.

As a sort of crude analogue with the theory set forth in §A, we might guess that w, u are further related by the formula:

$$w(x,y,t) = \chi_{u(x,t)}(y). \tag{38}$$

This equality says that "on the mesoscopic scale the velocity distribution is governed by the pseudo-Maxwellian, with macroscopic parameter $a = u(x, t)$ at each point $x \in \mathbb{R}^n$, time $t \geq 0$". It is remarkable that this rough interpretation can be made quite precise.

Theorem

(i) *Let u be a bounded entropy solution of*

$$u_t + \text{ div } \mathbf{F}(u) = 0 \text{ in } \mathbb{R}^n \times (0, \infty) \tag{39}$$

and define

$$w(x,y,t) = \chi_{u(x,t)}(y) \qquad (x \in \mathbb{R}^n,\ g \in \mathbb{R},\ t \geq 0). \tag{40}$$

Then

$$w \in C([0,\infty),\ L^1(\mathbb{R}^n \times \mathbb{R})) \cap L^\infty(\mathbb{R}^n_x \times (0,\infty),\ L^1(\mathbb{R}_y))$$

solves the kinetic equation

$$w_t + \mathbf{b}(y) \cdot D_x w = m_y \text{ in } \mathbb{R}^n \times \mathbb{R} \times (0,\infty) \tag{41}$$

for some nonnegative Radon measure m, supported in

$$\mathbb{R}^n \times [-R_0, R_0] \times (0,\infty),$$

where $R_0 = \|u\|_{L^\infty}$.

(ii) *Conversely, let* $w \in C([0,\infty);\ L^1(\mathbb{R}^n \times \mathbb{R})) \cap L^\infty(\mathbb{R}^n_x \times (0,\infty),\ L^1(\mathbb{R}_y))$ *solve* (41) *for some measure* m *as above. Assume also* w *has the form*

$$w = \chi_{u(x,t)}.$$

Then

$$u(x,t) = \int_{\mathbb{R}} w(x,y,t)dy \tag{42}$$

is an entropy solution of (39).

Proof. 1. First we prove (ii). Let $\Phi : \mathbb{R} \to \mathbb{R}$ be convex, with $\Phi(0) = 0$. Temporarily assume as well that Φ is C^2. Let $\psi \in C_c^\infty(\mathbb{R})$ satisfy

$$\begin{cases} 0 \le \psi \le 1,\ \psi \equiv 1 \text{ on } [-R_0, R_0] \\ \psi \equiv 0 \text{ on } \mathbb{R} - [-R_0 - 1, R_0 + 1]. \end{cases} \tag{43}$$

Take $v \in C_c^1(\mathbb{R}^n \times (0,\infty))$, $v \ge 0$. We employ

$$v(x,t)\Phi'(y)\psi(y) \tag{44}$$

as a test function in the definition of w as a weak solution of the transport equation (41):

$$\begin{array}{rcl} \int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}^n} w(v\Phi'\psi)_t & + & w\mathbf{b}(y) \cdot D_x(v\Phi'\psi)dxdydt \\ & = & \int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}^n} (v\Phi'\psi)_y dm. \end{array} \tag{45}$$

We must examine each term in this identity.

2. Now

$$\begin{array}{l} \int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}^n} w(v\Phi'\psi)_t dxdydt \\ = \int_0^\infty \int_{\mathbb{R}^n} v_t \left(\int_{\mathbb{R}} w\Phi'\psi dy \right) dxdt. \end{array}$$

By hypothesis $w = \chi_{u(x,t)}$, and therefore

$$\begin{array}{rcll} \int_{\mathbb{R}} w(x,y,t)\Phi'(y)\psi(y)dy & = & \int_{\mathbb{R}} \chi_{u(x,t)}(y)\Phi'(y)\psi(y)dy & \\ & = & \int_0^{u(x,t)} \Phi'(y)\psi(y)dy & \text{if } u(x,t) \ge 0 \\ & = & \Phi(u(x,t)), & \end{array} \tag{46}$$

since $\Phi(0) = 0$ and $\psi \equiv 1$ on $[0, u(x,t)]$. A similar computation is valid if $u(x,t) \le 0$. Hence

$$\begin{array}{l} \int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}^n} w(v\Phi'\psi_k)_t dxdydt \\ = \int_0^\infty \int_{\mathbb{R}^n} v_t \Phi(u) dxdt. \end{array} \tag{47}$$

Similarly,

$$\begin{aligned}&\int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}^n} w\mathbf{b}(y) \cdot D_x(v\Phi'\psi)dxdydt\\ &= \int_0^\infty \int_{\mathbb{R}^n} D_x v \cdot \left(\int_{\mathbb{R}} \mathbf{b}(y) w\Phi'\psi dy\right) dxdt.\end{aligned}$$

Now if $u(x,t) \geq 0$, then

$$\begin{aligned}\int_{\mathbb{R}} w\mathbf{b}(y)\Phi'\psi dy &= \int_0^{u(x,t)} \mathbf{b}(y)\Phi'(y)\psi(y)dy\\ &= \mathbf{\Psi}(u(x,t)),\end{aligned}$$

for

$$\mathbf{\Psi}(z) := \int_0^z \mathbf{b}(y)\Phi'(y)dy. \tag{48}$$

The same calculation is valid if $u(x,t) \leq 0$. Thus

$$\begin{aligned}&\int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}^n} w\mathbf{b}(y) \cdot D_x(v\Phi'\psi)dxdydt\\ &= \int_0^\infty \int_{\mathbb{R}^n} Dv \cdot \mathbf{\Psi}(u)dxdt.\end{aligned} \tag{49}$$

3. We investigate now the term on the right hand side of (45):

$$\begin{aligned}\int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}^n} (v\Phi'\psi)_y dm &= \int_0^\infty \int_{\mathbb{R}^n} \int_{\mathbb{R}} v(\Phi''\psi + \Phi'\psi')dm\\ &\geq \int_0^\infty \int_{\mathbb{R}^n} \int_{\mathbb{R}} v\Phi'\psi' dm,\end{aligned} \tag{50}$$

since $\Phi'' \geq 0, \psi, v \geq 0$. Additionally, since $\psi' \equiv 0$ on the support of m, we have

$$\int_0^\infty \int_{\mathbb{R}^n} \int_{\mathbb{R}} v\Phi'\psi' dm = 0. \tag{51}$$

4. Combine (45), (47), (49), (51), to conclude

$$\int_0^\infty \int_{\mathbb{R}^n} \Phi(u)v_t + \mathbf{\Psi}(u) \cdot Dv dxdt \geq 0 \tag{52}$$

for all v as above. An easy approximation removes the requirement that Φ be C^2. Thus for each entropy/entropy flux pair we have

$$\Phi(u)_t + \text{ div } \mathbf{\Psi}(u) \leq 0 \text{ in } \mathbb{R}^n \times (0,\infty)$$

in the weak sense, and consequently u is an entropy solution of (39).

5. Now we prove assertion (i) of the Theorem. Let u be a bounded entropy solution of $u_t + \text{ div } \mathbf{F}(u) = 0$ and *define*

$$w(x,y,t) := \chi_{u(x,t)}(y) \qquad (x \in \mathbb{R}^n,\ y \in \mathbb{R},\ t \geq 0). \tag{53}$$

Define also the distribution T on $\mathbb{R}^n \times \mathbb{R} \times (0,\infty)$ by

$$\langle T, \phi\rangle := -\int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}^n} w(\phi_t + \mathbf{b}(y)\cdot D_x\phi)dxdydt \tag{54}$$

for all $\phi \in C_c^\infty(\mathbb{R}^n \times \mathbb{R} \times (0,\infty))$. That is,

$$T = w_t + \mathbf{b}(y)\cdot D_x w \text{ in the distribution sense.} \tag{55}$$

Observe $T = 0$ off $\mathbb{R}^n \times [-R_0, R_0] \times (0,\infty)$, where $R_0 = \|u\|_{L^\infty}$.

Define now another distribution M by

$$\langle M, \phi\rangle := -\langle T, \int_{-\infty}^y \phi(x,z,t)dz\rangle \tag{56}$$

for ϕ as above. Then

$$T = \frac{\partial M}{\partial y} \text{ in the distribution sense.} \tag{57}$$

6. We now *claim* that

$$\langle M, \phi\rangle \geq 0 \tag{58}$$

for all $\phi \in C_c^\infty(\mathbb{R}^n \times \mathbb{R} \times (0,\infty))$ with $\phi \geq 0$.

To verify this, first suppose

$$\phi(x,y,t) = \alpha(x,t)\beta(y), \tag{59}$$

with

$$\begin{cases} \alpha \geq 0,\ \alpha \in C_c^\infty(\mathbb{R}^n \times (0,\infty)) \\ \beta \geq 0,\ \beta \in C_c^\infty(\mathbb{R}). \end{cases}$$

Take

$$\Phi(y) := \int_0^y \int_{-\infty}^z \beta(w)dwdz. \tag{60}$$

Then

$$\begin{aligned} \langle M, \phi\rangle &= \langle M, \alpha\beta\rangle \\ &= -\langle T, \alpha\Phi'\rangle \text{ by (56), (60)} \\ &= \textstyle\int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}^n} w[\alpha_t + \mathbf{b}(y)\cdot D_x\alpha]\Phi' dxdydt \text{ by (54)} \\ &= \textstyle\int_0^\infty \int_{\mathbb{R}^n} \int_{\mathbb{R}} \chi_u \Phi'[\alpha_t + \mathbf{b}(y)\cdot D_x\alpha]dydxdt \\ &= \textstyle\int_0^\infty \int_{\mathbb{R}^n} \Phi(u)\alpha_t + \mathbf{\Psi}(u)\cdot D_x\alpha dxdt, \end{aligned} \tag{61}$$

where

$$\mathbf{\Psi}' = \phi' \mathbf{a}.$$

The last equality results from calculations like those in steps 1,2 above. Now Φ is convex and so, since u is an entropy solution, the last term in (60) is nonnegative. Thus

$$\begin{cases} \langle M, \phi \rangle \geq 0 \text{ if } \phi(x,y,t) = \alpha(x,t)\beta(y), \\ \text{where } \alpha \geq 0,\ \beta \geq 0. \end{cases} \tag{62}$$

Next, take

$$\eta(x,y,t) = \lambda(x,t)\nu(y)$$

where λ, ν are smooth, nonnegative and have compact support. Assume also

$$\int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}^n} \eta dx dy dt = 1.$$

Let $\eta_\varepsilon(\cdot) = \frac{1}{\varepsilon^{n+2}} \eta(\cdot/\varepsilon)$, and then, given $\phi \in C_c^\infty(\mathbb{R}^n \times \mathbb{R} \times (0,\infty))$, $\phi \geq 0$, set

$$\begin{aligned} \phi_\varepsilon(x,y,t) &= (\eta_\varepsilon * \phi)(x,y,t) \\ &= \int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}^n} \lambda_\varepsilon(x-\bar{x}, t-\bar{t}) \nu_\varepsilon(y-\bar{y}) \phi(\bar{x},\bar{y},\bar{t}) d\bar{x} d\bar{y} d\bar{t}. \end{aligned}$$

We have

$$\begin{aligned} \langle M, \phi_\varepsilon \rangle &= \int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}^n} \langle M, \lambda_\varepsilon \nu_\varepsilon \rangle \phi(\bar{x},\bar{y},\bar{t}) d\bar{x} d\bar{y} d\bar{t} \\ &\geq 0, \end{aligned}$$

owing to (62). Send $\varepsilon \to 0$ to establish the claim (58).

7. Finally we recall that (56) implies M is represented by a nonnegative Radon measure. That is, there exists m as stated in the Theorem such that

$$\langle M, \phi \rangle = \int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}} \phi dm.$$

(See e.g. [E-G].) Thus

$$w_t + \mathbf{b}(y) \cdot D_x w = T = \frac{\partial M}{\partial y} = m_y$$

in the distribution sense. □

Remark. For each entropy/entropy flux pair

$$\Phi(u)_t + \text{ div } \mathbf{\Psi}(u) \leq 0$$

in the distribution sense, and so—as above—we can represent

$$\Phi(u)_t + \text{ div } \mathbf{\Psi}(u) = -\gamma^\Phi$$

where γ^Φ is a nonnegative Radon measure on $\mathbb{R}^n \times (0,\infty)$, *depending on* Φ. This measure is supported outside of any open regions where u is C^1, and so records the "change of the entropy $\Phi(u)$ along the shocks and other places where u is not smooth".

The measure m on the right hand side of the kinetic equation (41) for $w = \chi_u$ somehow records simultaneously the information encoded in γ^Φ for *all* the entropies Φ. □

5. A hydrodynamical limit

To illustrate the usefulness of the kinetic formulation of the conservation law introduced in §4, we consider in this section the problem of understanding the limit as $\varepsilon \to 0$ of solutions of the *scaled transport* equation

$$w_t^\varepsilon + \mathbf{b}(y) \cdot D_x w^\varepsilon = \frac{1}{\varepsilon}(\chi_{u^\varepsilon} - w^\varepsilon) \text{ in } \mathbb{R}^n \times \mathbb{R} \times (0,\infty) \tag{63}$$

where

$$u^\varepsilon(x,t) := \int_{\mathbb{R}} w^\varepsilon(x,y,t)dy. \tag{64}$$

This is a nonlocal PDE for the unknown w^ε.

Physical interpretation. We may think of (63) as a scaled, simplified version of Boltzmann's equation, the parameter ε being a crude approximation to the *mean free path length* between particle collisions. The right hand side of (63) is a sort of analogue of the collision operator $Q(\cdot,\cdot)$. If we similarly rescale Boltzmann's equation

$$f_t^\varepsilon + v \cdot D_x f^\varepsilon = \frac{1}{\varepsilon} Q(f^\varepsilon, f^\varepsilon)$$

and send $\varepsilon \to 0$, we may expect the particle density $f^\varepsilon(\cdot, v, \cdot)$ to approach a Maxwellian distribution, controlled by the macroscopic parameters $\rho(x,t), \mathbf{v}(x,t), \theta(x,t)$, which in turn should satisfy macroscopic PDE. See for instance Bardos–Golse–Levermore [B-G-L] for more on this. This is called a *hydrodynamical limit*. □

Our scaled problem (63), (64) is a vastly simplified variant, for which it is possible to understand rigorously the limit $\varepsilon \to 0$. First let us adjoin to (63), (64) the initial condition

$$w^\varepsilon = \chi_g \text{ on } \mathbb{R}^n \times \mathbb{R} \times \{t = 0\}, \tag{65}$$

where $g : \mathbb{R}^n \to \mathbb{R}$ is a given, smooth function, with compact support.

Theorem *As* $\varepsilon \to 0$,

$$w^\varepsilon \overset{*}{\rightharpoonup} w \text{ weakly} * \text{ in } L^\infty(\mathbb{R}^n \times \mathbb{R} \times (0,\infty)), \tag{66}$$

where w solves

$$\text{(67)}\qquad \begin{cases} w_t + \mathbf{b}(y)\cdot D_x w &= m_y \\ w &= \chi_u \text{ in } \mathbb{R}^n\times\mathbb{R}\times(0,\infty) \\ w &= \chi_g \text{ on } \mathbb{R}^n\times\mathbb{R}\times\{t=0\}, \end{cases}$$

for m a nonnegative Radon measure and u the unique entropy solution of

$$\text{(68)}\qquad \begin{cases} u_t + \text{ div } \mathbf{F}(u) &= 0 \text{ on } \mathbb{R}^n\times(0,\infty) \\ u &= g \text{ on } \mathbb{R}^n\times\{t=0\}. \end{cases}$$

We say the conservation law (68) is the *hydrodynamical limit* of the scaled kinetic equations (63) as $\varepsilon\to 0$.

Proof (Outline). 1. It is shown in [P-T] that

$$\text{(69)}\qquad \begin{cases} \{u^\varepsilon\}_{0<\varepsilon\le 1} \text{ is strongly precompact in} \\ L^1_{\text{loc}}(\mathbb{R}^n\times[0,\infty)), \end{cases}$$

and further

$$\text{(70)}\qquad \begin{cases} |w^\varepsilon|\le 1 \text{ a.e.}, \\ w^\varepsilon\ge 0 \text{ on } \{y\ge 0\},\ w^\varepsilon\le 0 \text{ on } \{y\le 0\}. \\ \text{supt}(w^\varepsilon)\subset\mathbb{R}^n\times[-R_0,R_0]\times(0,\infty), \end{cases}$$

where $R_0 = \|g\|_{L^\infty}$. We will use these facts below.

2. We now *claim* that we can write

$$\text{(71)}\qquad \frac{1}{\varepsilon}(\chi_{u^\varepsilon} - w^\varepsilon) = m^\varepsilon_y,$$

for some nonnegative function m^ε supported in $\mathbb{R}^n\times[-R_0,R_0]\times(0,\infty)$. To confirm this, fix $-R_0\le a\le R_0$ and assume $h\in L^\infty(\mathbb{R})$ satisfies

$$\text{(72)}\qquad \begin{cases} \text{supt}(h)\subset[-R_0,R_0], \\ -1\le h\le 0 \text{ if } y\le 0 \\ 0\le h\le 1 \text{ if } y\ge 0 \\ \int_{\mathbb{R}} h dy = a \end{cases}$$

Then

$$\text{(73)}\qquad \chi_a(y) - h(y) = q'(y) \qquad \text{(a.e. } y\in\mathbb{R})$$

for

$$q(y) := \int_{-\infty}^{y} \chi_a(z) = h(z)dz.$$

Recall that

$$\chi_a(z) = \begin{cases} 1 & \text{if } 0 \le z \le a \\ -1 & \text{if } a \le z \le 0 \\ 0 & \text{otherwise.} \end{cases}$$

Thus if $a \ge 0$, we deduce from (72), (73) that

$$\begin{cases} q' \ge 0 & \text{for a.e. } -\infty < y < a \\ q' \le 0 & \text{for a.e. } a < y < \infty \end{cases}$$

and the same inequalities are true if $a \le 0$. Furthermore $q(-R_0) = 0$ and

$$\begin{aligned} q(R_0) &= \textstyle\int_{-R_0}^{R_0} \chi_a(z) - h(z)dz \\ &= a - \textstyle\int_{-\infty}^{\infty} h dz = 0. \end{aligned}$$

Hence

$$q \ge 0 \text{ on } \mathbb{R}. \tag{74}$$

3. Recall (72) and apply the results in step 2 to

$$\begin{aligned} h(y) &= w^\varepsilon(x,y,t), \\ a &= u^\varepsilon(x,t) = \textstyle\int_{\mathbb{R}} w^\varepsilon(x,y,t)dy. \end{aligned}$$

According to (70), this choice of h satisfies conditions (72). Then (73), (74) say

$$\frac{1}{\varepsilon}(\chi_{u^\varepsilon} - w^\varepsilon) = m_y^\varepsilon,$$

where

$$\operatorname{supt}(m^\varepsilon) \subset [-R_0, R_0],\ m^\varepsilon \ge 0$$

for each (x,t). This is assertion (71).

4. Next we assert:

$$\sup_{0<\varepsilon\le 1} \|m_\varepsilon\|_{L^1(\mathbb{R}^n\times\mathbb{R}\times(0,\infty))} < \infty. \tag{75}$$

A formal calculation leading to (75) is this:

$$\begin{aligned}
\int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}^n} m^\varepsilon dxdydt &= \int_0^\infty \int_{\mathbb{R}^n} \int_{\mathbb{R}} m^\varepsilon(y)_y dydxdt \\
&= -\int_0^\infty \int_{\mathbb{R}^n} \int_{\mathbb{R}} m^\varepsilon_y y dydxdt \\
&= -\int_0^\infty \int_{\mathbb{R}^n} \int_{\mathbb{R}} (w^\varepsilon_t + \mathbf{b}(y) \cdot D_x w^\varepsilon) y dydxdt \\
&= \int_{\mathbb{R}^n} \int_{\mathbb{R}} w^\varepsilon(x,y,0) y dydx \\
&= \int_{\mathbb{R}^n} \int_{\mathbb{R}} \chi_{g(x)}(y) y dydx \text{ by (65)} \\
&= \int_{\mathbb{R}^n} \tfrac{g^2}{2} dx < \infty.
\end{aligned}$$

We omit the detailed proof of (75).

5. Employing now (69), (70), (75) we extract a sequence $\varepsilon_r \to 0$ so that

$$\begin{cases}
w^{\varepsilon_r}_{\varepsilon_r} \overset{*}{\rightharpoonup} w & \text{weakly } * \text{ in } L^\infty \\
u_{\varepsilon_r} \to u & \text{strongly in } L^1_{\text{loc}} \\
m^{\varepsilon_r} \rightharpoonup m & \text{weakly } * \text{ as measures.}
\end{cases}$$

Hence

$$w_t + \mathbf{b}(y) \cdot D_x w = m_y \text{ in } \mathbb{R}^n \times \mathbb{R} \times (0,\infty) \tag{76}$$

in the weak sense. Furthermore

$$\chi_{u^\varepsilon} - w^\varepsilon = \varepsilon m^\varepsilon y;$$

and so for each $\phi \in C_c^\infty(\mathbb{R}^n \times \mathbb{R} \times (0,\infty))$,

$$\int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}^n} \phi(\chi_{u^\varepsilon} - w^\varepsilon) dxdydt = -\varepsilon \int_0^\infty \int_{\mathbb{R}^n} \int_{\mathbb{R}} \phi_y dm^\varepsilon \to 0.$$

Consequently

$$\chi_{u^{\varepsilon_r}} \overset{*}{\rightharpoonup} w \text{ weakly } * \text{ in } L^\infty. \tag{77}$$

Now

$$\chi_{u^{\varepsilon_r}}(y) = \begin{cases}
1 & \text{if } 0 \le y \le u^{\varepsilon_r} \\
-1 & \text{if } u^{\varepsilon_r} \le y \le 0 \\
0 & \text{otherwise,}
\end{cases}$$

and so

$$\int_{\mathbb{R}} |\chi_{u^{\varepsilon_r}} - \chi_u| dy = |u^{\varepsilon_r} - u|.$$

Since $u^{\varepsilon_r} \to u$ strongly in L^1_{loc}, we see

$$\chi_{u^{\varepsilon_r}} \to \chi_u \text{ in } L^1_{\text{loc}}.$$

Thus

$$w = \chi_u.$$

Hence (67) holds and so, according to the kinetic formulation in §4, u solves the conservation law (68). □

C. Systems of conservation laws

A *system of conservation laws* is written

$$\mathbf{u}_t + \text{ div } \mathbf{F}(\mathbf{u}) = 0 \text{ in } \mathbb{R}^n \times (0,\infty), \tag{1}$$

where the unknown is

$$\mathbf{u} : \mathbb{R}^n \times [0,\infty) \to \mathbb{R}^m, \ \mathbf{u} = (u^1, \dots, u^m)$$

and

$$\mathbf{F} : \mathbb{R}^m \to \mathbb{M}^{m\times n}, \ \mathbf{F} = \begin{pmatrix} F_1^1 & \dots & F_n^1 \\ \vdots & & \vdots \\ F_1^m & \dots & F_n^m \end{pmatrix}_{m\times n}$$

is given.

Notation. (i) We can rewrite (1) into the nondivergence form

$$\mathbf{u}_t + B(\mathbf{u})^T : D\mathbf{u} = 0 \text{ in } \mathbb{R}^n \times (0,\infty) \tag{2}$$

for

$$\mathbf{B} = D\mathbf{F}, \ \mathbf{B} : \mathbb{R}^m \to L(\mathbb{R}^m, \mathbb{M}^{m\times n}).$$

We sometimes write $\mathbf{F} = \mathbf{F}(z)$, $\mathbf{B} = \mathbf{B}(z)$ for $z \in \mathbb{R}^m$. □

(ii) In terms of the components of $\mathbf{u}$, (1) says

$$u_t^k + \sum_{i=1}^n (F_i^k(\mathbf{u}))_{x_i} = 0 \qquad (k = 1, \dots, m) \tag{3}$$

and (2) means

$$u_t^k + \sum_{i=1}^n \sum_{l=1}^m \frac{\partial F_i^k(\mathbf{u})}{\partial z_l} u_{x_i}^l = 0 \qquad (k = 1, \dots, m). \tag{4}$$

□

We are interested in properly formulating the initial value problem

$$\begin{cases} \mathbf{u}_t + \text{ div } \mathbf{F}(\mathbf{u}) &= 0 \text{ in } \mathbb{R}^n \times (0,\infty) \\ \mathbf{u} &= \mathbf{g} \text{ on } \mathbb{R}^n \times \{t=0\}, \end{cases} \tag{5}$$

where

$$\mathbf{g} : \mathbb{R}^n \to \mathbb{R}^m,\ \mathbf{g} = (g^1, \dots, g^m)$$

is given.

1. Entropy conditions

Definition. We say $\mathbf{u} \in L^1_{\text{loc}}(\mathbb{R}^n \times (0,\infty);\ \mathbb{R}^m)$ is an *integral solution* of (5) provided

$$\int_0^\infty \int_{\mathbb{R}^n} \mathbf{u} \cdot \mathbf{v}_t + \mathbf{F}(\mathbf{u}) : D\mathbf{v} dx dt + \int_{\mathbb{R}^n} \mathbf{g} \cdot \mathbf{v}(\cdot, 0) dx = 0 \tag{6}$$

for each $\mathbf{v} \in C_c^1(\mathbb{R}^n \times [0,\infty);\ \mathbb{R}^m)$.

Notation. We write $\mathbf{v} = (v^1, \dots, v^m)$,

$$\begin{aligned} D\mathbf{v} &= \begin{pmatrix} v^1_{x_1} & \dots & v^1_{x_n} \\ v^m_{x_1} & \dots & v^m_{x_n} \end{pmatrix}, \\ \mathbf{F}(\mathbf{u}) : D\mathbf{v} &= \textstyle\sum_{k=1}^m \sum_{i=1}^n F_i^k(u) v^k_{x_i}. \end{aligned}$$

□

As for scalar conservation laws this is an inadequate notion of solution, and so we introduce this additional

Definition. We call $(\Phi, \mathbf{\Psi})$ an *entropy/entropy flux pair* for the conservation law (1) provided

(i) $\Phi : \mathbb{R}^m \to \mathbb{R}$ is convex

and

(ii) $\mathbf{\Psi} : \mathbb{R}^m \to \mathbb{R}^n$, $\mathbf{\Psi} = (\Psi^1, \dots, \Psi^n)$

satisfies

$$D\mathbf{\Psi} = \mathbf{B} D\Phi. \tag{7}$$

Notation. The identity (7) means:

$$\Psi^i_{z_k} = \sum_{l=1}^m \frac{\partial F_i^l}{\partial z_k} \Phi_{z_l} \qquad (1 \le i \le n,\ 1 \le k \le m). \tag{8}$$

Motivation. Suppose $\mathbf{u}$ is a C^1 solution of (1) in some region of $\mathbb{R}^n \times (0,\infty)$. Then

$$\Phi(\mathbf{u})_t + \text{ div } \mathbf{\Psi}(\mathbf{u}) = 0 \tag{9}$$

there. Indeed, we compute:

$$\begin{aligned}
\Phi(\mathbf{u})_t + \text{ div } \mathbf{\Psi}(\mathbf{u}) &= \textstyle\sum_{k=1}^m \Phi_{z_k}(\mathbf{u}) u_t^k \\
&\quad + \textstyle\sum_{k=1}^m \sum_{i=1}^n \Psi^i_{z_k}(\mathbf{u}) u^k_{x_i} \\
&= -\textstyle\sum_{k,l=1}^m \sum_{i=1}^n \Phi_{z_k}(\mathbf{u}) \frac{\partial F_i^k(\mathbf{u})}{\partial z_l} u^l_{x_i} \\
&\quad + \textstyle\sum_{k=1}^m \sum_{i=1}^n \Psi^i_{z_k}(\mathbf{u}) u^k_{x_i} \text{ according to (4)} \\
&= \textstyle\sum_{k=1}^m \sum_{i=1}^n \left(-\sum_{l=1}^m \Phi_{z_l}(\mathbf{u}) \frac{\partial F_i^l(\mathbf{u})}{\partial z_k} + \Psi^i_{z_k}(\mathbf{u}) \right) u^k_{x_i} \\
&= 0, \text{ owing to (8).}
\end{aligned}$$

□

Unlike the situation for scalar conservation laws (i.e. $m = 1$), there need not exist any entropy/entropy flux pairs for a given system of convservation laws. For physically derived PDE, on the other hand, we can hope to discern at least some such pairs.

2. Compressible Euler equations in one space dimension

We return to §A.1 and consider now the compressible, isentropic Euler equations *in one space dimension*. According to (6) in §A.1, the relevant PDE are

$$\begin{cases} \rho_t + (\rho v)_x = 0 \\ (\rho v)_t + (\rho v^2 + p)_x = 0 \end{cases} \text{ in } \mathbb{R}^1 \times (0,\infty), \tag{10}$$

where ρ is the density, v the velocity and

$$p = p(\rho) \tag{11}$$

is the pressure. Observe that (10) is of the form

$$\mathbf{u}_t + (\mathbf{F}(\mathbf{u}))_x = 0$$

for $m = 2$,

$$\begin{cases} \mathbf{u} = (\rho, \rho v) \\ \mathbf{F} = (z_2, z_2^2/z_1 + p(z_1)). \end{cases} \tag{12}$$

Remark. We have

$$\mathbf{B} = D\mathbf{F} = \begin{pmatrix} 0 & 1 \\ -z_2^2/z_1^2 + p'(z_1) & 2z_2/z_1 \end{pmatrix}.$$

The eigenvalues of $\mathbf{B}$ are

$$\lambda_\pm = \frac{z_2}{z_1} \pm (p'(z_1))^{1/2}$$

assuming

$$p' > 0. \tag{13}$$

Reverting to physical variables, we see

$$\lambda_\pm = v \pm (p'(\rho))^{1/2}.$$

It follows that the *speed of sound* for isentropic flow is

$$p'(\rho)^{1/2}.$$

□

a. Computing entropy/entropy flux pairs

We attempt now to discover entropy/entropy flux pairs (Φ, Ψ), where to simplify subsequent calculations we look for Φ, Ψ as functions of (ρ, v) (and not $(u^1, u^2) = (\rho, \rho v)$). Thus we seek

$$\Phi = \Phi(\rho, v), \ \ \Psi = \Psi(\rho, v)$$

such that

$$\text{the mapping } (\rho, \rho v) \mapsto \Phi \text{ is convex} \tag{14}$$

and

$$\begin{cases} \Phi_t + \Psi_x = 0 \text{ in any} \\ \text{region where } (\rho, v) \text{ are } C^1\text{-solutions of (10).} \end{cases} \tag{15}$$

So let us assume (ρ, v) solve (10), which we recast into nondivergence form:

$$\begin{cases} \rho_t + \rho_x v + \rho v_x &= 0 \\ v_t + v v_x &= -\frac{1}{\rho} p_x = -p' \frac{\rho_x}{\rho}. \end{cases} \tag{16}$$

Observe that the second line here is just the second line of formula (1) from §A.1. So if $\Phi = \Phi(\rho, v)$, $\Psi = \Psi(\rho, v)$, we can compute:

$$\begin{aligned}\Phi_t + \Psi_x &= \Phi_\rho \rho_t + \Phi_v v_t + \Psi_\rho \rho_x + \Psi_v v_x \\ &= \Phi_\rho(-\rho_x v - \rho v_x) + \Phi_v\left(-v v_x - p'\tfrac{\rho_x}{\rho}\right) \\ &\quad + \Psi_\rho \rho_x + \Psi_v v_x \\ &= \rho_x\left[\Psi_\rho - v\Phi_\rho - \tfrac{p'}{\rho}\Phi_v\right] \\ &\quad + v_x[\Psi_v - \rho\Phi_\rho - v\Phi_v].\end{aligned}$$

Consequently, $\Phi_t + \Psi_x \equiv 0$ for all smooth solutions (ρ, v) of (15) if and only if

$$\left\{\begin{array}{rcl}\Psi_\rho &=& v\Phi_\rho + \frac{p'}{\rho}\Phi_v \\ \Psi_v &=& \rho\Phi_\rho + v\Phi_v.\end{array}\right. \tag{17}$$

We proceed further by noting $\Psi_{\rho v} = \Psi_{v\rho}$:

$$\left(v\Phi_\rho + \frac{p'}{\rho}\Phi_v\right)_v = (\rho\Phi_\rho + v\Phi_v)_\rho.$$

Hence

$$\Phi_\rho + v\Phi_{\rho v} + \frac{p'}{\rho}\Phi_{vv} = \Phi_\rho + \rho\Phi_{\rho\rho} + v\Phi_{v\rho},$$

and consequently

$$\Phi_{\rho\rho} = \frac{p'(\rho)}{\rho^2}\Phi_{vv} \qquad (\rho > 0,\ v \in \mathbb{R}). \tag{18}$$

In summary, if Φ solves (18) and we compute Ψ from (17), then (Φ, Ψ) satisfies $\Phi_t + \Psi_x = 0$, whenever (ρ, v) are smooth solutions of Euler's equations (10). Since $p' > 0$, (18) is a linear nonhomogeneous wave equation.

Definition. Φ is called a *weak entropy function* if Φ solves (18), with the initial conditions

$$\Phi = 0,\ \Phi_\rho = g \text{ on } \mathbb{R} \times \{\rho > 0\}, \tag{19}$$

for some given $g : \mathbb{R} \to \mathbb{R}$, $g = g(v)$.

To go further, let us take from §A.1 the explicit equation of state

$$p(\rho) = \kappa\rho^\gamma, \text{ where } \kappa = \frac{(\gamma-1)^2}{4\gamma},\ \gamma > 1 \tag{20}$$

the constant κ so selected to simplify the algebra.

Lemma (i) *The solution of* (17), (18) *for*

$$g = \delta_{\{0\}} = \text{ Dirac mass at the origin}$$

is

$$\chi(\rho, v) = (\rho^{\gamma-1} - v^2)_+^{\lambda},\ \lambda = \frac{3-\gamma}{2(\gamma-1)}. \tag{21}$$

(ii) *The general solution of* (17), (18) *is*

$$\Phi(\rho, v) = \int_{\mathbb{R}} g(y)\chi(\rho, y-v)dy \qquad (\rho > 0,\ v \in \mathbb{R}). \tag{22}$$

(iii) *Furthermore,* Φ *defined by* (21) *is convex in* $(\rho, \rho v)$ *if and only if* g *is convex.*
(iv) *The entropy flux* Ψ *associated with* Φ *is*

$$\Psi(\rho, v) = \int_{\mathbb{R}} g(y)(\theta y + (1-\theta)v)\chi(\rho, y-v)dy \tag{23}$$

for $\theta = \frac{\gamma-1}{2}$.

See [L-P-T2] for proof. We will momentarily see that we can regard χ as a sort of pseudo-Maxwellian, parameterized by the macroscopic parameters ρ, v.

Example. Take $g(v) = v^2$. Then

$$\begin{aligned} \Phi(\rho, v) &= \textstyle\int_{\mathbb{R}} y^2(\rho^{\gamma-1} - (y-v)^2)^{\lambda} + dy \\ &= \tfrac{1}{2}\rho v^2 + \tfrac{k}{\gamma-1}\rho^{\gamma}. \end{aligned} \tag{24}$$

The term $\frac{1}{2}\rho v^2$ is the density of the kinetic energy, and $\frac{k}{\gamma-1}\rho^{\gamma}$ is the density of the internal energy. Hence Φ is the *energy density*. If $(\rho, \rho v)$ is an entropy solution of (10), then

$$\Phi_t + \Psi_x \leq 0,$$

and so

$$\sup_{t\geq 0} \int_{\mathbb{R}} \frac{1}{2}\rho(x,t)v^2(x,t) + \frac{k}{\gamma-1}\rho^{\gamma}(x,t)dx < \infty, \tag{25}$$

provided the initial conditions satisfy this bound. □

b. Kinetic formulation

Theorem *Let* $(\rho, \rho v) \in L^\infty((0,\infty);\ L^1(\mathbb{R}, \mathbb{R}^2))$ *have finite energy and suppose* $\rho \geq 0$ *a.e. Then* $(\rho, \rho v)$ *is an entropy solution of Euler's equations*

$$\left\{ \begin{array}{rcl} \rho_t + (\rho v)_x & = & 0 \\ & & \\ (\rho v)_t + (\rho v^2 + p)_x & = & 0 \end{array} \right. \quad in\ \ \mathbb{R} \times (0,\infty) \tag{26}$$

if and only if there exists a nonpositive *measure* m *on* $\mathbb{R} \times \mathbb{R} \times (0,\infty)$ *such that*

$$w = \chi(\rho, y - v) \qquad (\rho = \rho(x,t),\ v = v(x,t),\ y \in \mathbb{R}) \tag{27}$$

satisfies

$$w_t + [(\theta y + (1-\theta)v)w]_x = m_{yy} \ in\ \mathbb{R} \times \mathbb{R} \times (0,\infty). \tag{28}$$

We call (27), (28) a *kinetic formulation* of (26).

Proof. 1. As in §B.4 define the distributions

$$T = w_t + [(\theta y + (1-\theta)v)w]_x \tag{29}$$

and

$$\frac{\partial^2 M}{\partial y^2} = T. \tag{30}$$

2. Take Φ, Ψ to be a weak entropy/entropy flux pair as above. That is,

$$\begin{array}{rcl} \Phi(\rho, v) & = & \int_{\mathbb{R}} g(y)\chi(\rho, y - v)dy \\ \Psi(\rho, v) & = & \int_{\mathbb{R}} g(y)(\theta y + (1-\theta)v)\chi(\rho, y - v)dy. \end{array}$$

Then

$$\Phi_t + \Psi_x = \int_{\mathbb{R}} g(y)(w_t + [(\theta y + (1-\theta)v)w]_x)dy. \tag{31}$$

Suppose now

$$\phi(x, y, t) = \alpha(x,t)\beta(y)$$

where

$$\left\{ \begin{array}{l} \alpha \geq 0,\ \alpha \in C_c^\infty \\ \beta \geq 0,\ \beta \in C_c^\infty. \end{array} \right.$$

Take g so that

$$g'' = \beta. \tag{32}$$

Then (30) implies

$$\begin{aligned} -\int_0^\infty \int_{\mathbb{R}} \Phi\alpha_t + \Phi\alpha_x dxdt &= \int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}} \alpha g(w_t + [(\theta y + (1-\theta)v)w]_x) dxdydt \\ &= \langle T, \alpha g\rangle \\ &= \langle M, \alpha\beta\rangle \text{ by (29), (31)} \\ &= \langle M, \phi\rangle. \end{aligned}$$

3. Now if $(\rho, \rho v)$ is an entropy solution, then

$$\int_0^\infty \int_{\mathbb{R}} \Phi\alpha_t + \Psi\alpha_x dxdt \geq 0 \tag{33}$$

since $\alpha \geq 0$, and thus $\langle M, \phi\rangle \leq 0$. This holds for all $\phi = \alpha\beta$ as above and so, as in §B.4,

$$\langle M, \phi\rangle \leq 0 \text{ for all } \phi \in C_c^\infty,\ \phi \geq 0. \tag{34}$$

Thus M is represented by a nonpositive measure m. Conversely if (33) holds, then (32) is valid for all $\alpha \geq 0$, $\alpha \in C_c^1$.

4. Lastly note the estimate

$$\begin{aligned} \int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}} dm &= \tfrac{1}{2} \int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}} (y^2)_{yy} dm \\ &= \tfrac{1}{2} \int_0^\infty \int_{\mathbb{R}} \int_{\mathbb{R}} y^2 [w_t + [(\theta y + (1-\theta)v)w]_x dxdydt \\ &= \tfrac{1}{2} \int_0^\infty \int_{\mathbb{R}} \Phi_t + \Psi_x dxdt \\ &= \tfrac{1}{2} \int_{\mathbb{R}} \Phi(\rho(\cdot,0), v(\cdot,0)) dx \\ &= \tfrac{1}{2} \int_{\mathbb{R}} \tfrac{1}{2}\rho(\cdot,0)v(\cdot,0)^2 + \tfrac{k}{\gamma-1}\rho(\cdot,0)^\gamma dx \\ &< \infty. \end{aligned}$$

□

See Lions–Perthame–Tadmor [L-P-T2] and Lions–Perthame–Souganidis [L-P-S] for remarkable applications.

CHAPTER 6: Hamilton–Jacobi and related equations

A. Viscosity solutions

A PDE of the form

$$u_t + H(Du) = 0 \text{ in } \mathbb{R}^n \times (0,\infty) \tag{1}$$

is called a *Hamilton–Jacobi equation*. The unknown is

$$u : \mathbb{R}^n \times [0,\infty) \to \mathbb{R}$$

and the *Hamiltonian*

$$H : \mathbb{R}^n \to \mathbb{R}$$

is a given continuous function. Here $Du = (D_x u) = (u_{x_1}, \dots, u_{x_n})$.

In this short chapter we introduce the notion of *viscosity solutions* of (1), which are defined in terms of various inequalities involving smooth test functions. The relevant theory will not seem to have anything much to do with our ongoing themes concerning entropy and PDE, but connections will be established later, in Chapter VIII.

Following Crandall–Lions [C-L] and [C-E-L] let us make the following

Definition. A bounded uniformly continuous function u is called a *viscosity solution* of (1) provided for each $v \in C^\infty(\mathbb{R}^n \times (0,\infty))$

$$\begin{cases} \text{if } u - v \text{ has a local } \textit{maximum} \text{ at a} \\ \text{point } (x_0, t_0) \in \mathbb{R}^n \times (0,\infty), \\ \text{then } v_t(x_0,t_0) + H(Dv(x_0,t_0)) \le 0 \end{cases} \tag{2}$$

and

$$\begin{cases} \text{if } u - v \text{ has a local } \textit{minimum} \text{ at a} \\ \text{point } (x_0, t_0) \in \mathbb{R}^n \times (0,\infty), \\ \text{then } v_t(x_0,t_0) + H(Dv(x_0,t_0)) \ge 0. \end{cases} \tag{3}$$

Motivation. If u happens to be a C^1 solution of (1) in some region of $\mathbb{R}^n \times (0,\infty)$, then in fact

$$v_t(x_0,t_0) + H(Dv(x_0,t_0)) = 0$$

at any point in that region where $u - v$ has a local maximum or minimum. This follows since $u_t = v_t$, $Du = Dv$ at such a point.

The interest in (2), (3) is consequently the possibility of the inequalities holding at points where u is not C^1. This is all obviously some kind of vague analogue of the theory from Chapter V. As in that chapter let us motivate (2), (3) by the vanishing viscosity method. So fix $\varepsilon > 0$ and consider the regularized PDE

$$u_t^\varepsilon + H(Du^\varepsilon) = \varepsilon \Delta u^\varepsilon \text{ in } \mathbb{R}^n \times (0, \infty). \tag{4}$$

Let us assume that as $\varepsilon \to 0$,

$$u^\varepsilon \to u \text{ locally uniformly} \tag{5}$$

and further suppose for some $v \in C^\infty$ that $u - v$ has a *strict* local maximum at some point $(x_0, t_0) \in \mathbb{R}^n \times (0, \infty)$. Then $u - v$ has a local maximum at a nearby point $(x_\varepsilon, t_\varepsilon)$, with

$$(x_\varepsilon, t_\varepsilon) \to (x_0, t_0) \text{ as } \varepsilon \to 0. \tag{6}$$

As v and our solution u^ε of the regularized problem (4) are smooth, we have

$$u_t^\varepsilon = v_t, \ Du^\varepsilon = Dv, \ D^2 u^\varepsilon \leq D^2 v \text{ at } (x_\varepsilon, t_\varepsilon), \tag{7}$$

the third expression recording the ordering of symmetric matrices. Then

$$\begin{aligned} v_t(x_\varepsilon, t_\varepsilon) + H(Dv(x_\varepsilon, t_\varepsilon)) &= u_t^\varepsilon(x_\varepsilon, t_\varepsilon) + H(Du^\varepsilon(x_\varepsilon, t_\varepsilon)) \text{ by (7)} \\ &= \varepsilon \Delta u^\varepsilon(x_\varepsilon, t_\varepsilon) \text{ by (4)} \\ &\leq \varepsilon \Delta v(x_\varepsilon, t_\varepsilon) \text{ by (7)}. \end{aligned}$$

Let $\varepsilon \to 0$ and recall (6):

$$v_t(x_0, t_0) + H(Dv(x_0, t_0)) \leq 0.$$

It is easy to modify this proof if $u - v$ has a local maximum which is not strict at (x_0, t_0). A similar proof shows that the reverse inequality holds should $u - v$ have a local minimum at a point (x_0, t_0).

Hence if the u^ε (or a subsequence) converge locally uniformly to a limit u, then u is a viscosity solution of (1). This construction by the vanishing viscosity method accounts for the name.[3] □

We will not develop here the theory of viscosity solutions, other than to state the fundamental theorem of Crandall–Lions:

Theorem *Assume that $u, \hat{u}$ are viscosity solutions of*

$$\begin{cases} u_t + H(Du) = 0 \text{ in } \mathbb{R}^n \times (0, \infty) \\ u = g \text{ on } \mathbb{R}^n \times \{t = 0\} \end{cases} \tag{8}$$

[3] In fact, Crandall and Lions originally considered the name "entropy solutions".

and

$$\text{(9)}\qquad \begin{cases} \hat{u}_t + H(D\hat{u}) &= 0 \text{ in } \mathbb{R}^n \times (0,\infty) \\ \hat{u} &= \hat{g} \text{ on } \mathbb{R}^n \times \{t=0\}. \end{cases}$$

Then

$$\|u(\cdot,t) - \hat{u}(\cdot,t)\|_{L^\infty(\mathbb{R}^n)} \le \|u(\cdot,s) - \hat{u}(\cdot,s)\|_{L^\infty(\mathbb{R}^n)}$$

for each $0 \le s \le t$.

In particular a *viscosity solution of the initial value problem* (8) *is unique*. See [C-E-L] for proof (cf. also [E1, §10.2]).

B. Hopf–Lax formula

For use later we record here a representation formula for the viscosity solution of

$$\text{(1)}\qquad \begin{cases} u_t + H(Du) &= 0 \text{ in } \mathbb{R}^n \times (0,\infty) \\ u &= g \text{ on } \mathbb{R}^n \times \{t=0\}, \end{cases}$$

in the special case that

$$\text{(2)}\qquad H : \mathbb{R}^n \to \mathbb{R} \text{ is convex}$$

and

$$\text{(3)}\qquad g : \mathbb{R}^n \to \mathbb{R} \text{ is bounded, Lipschitz.}$$

We have then the *Hopf–Lax formula*:

$$u(x,t) = \inf_{y \in \mathbb{R}^n} \left\{ tL\left(\frac{x-y}{t}\right) + g(y) \right\} \qquad (x \in \mathbb{R}^n,\ t \ge 0)$$

for the unique viscosity solution of (1). Here L is the Legendre transform of H:

$$L(q) = \sup_{p \in \mathbb{R}^n} \{p \cdot q - H(p)\}.$$

See [E1, §10.3.4] for a proof. We will invoke this formula in §VIII.C.

C. A diffusion limit

In Chapter VIII we will employ viscosity solution methods to study several asymptotic problems, involving—as we will see—entropy considerations. As these developments must wait, it is appropriate to include here a rather different application. We introduce for each

$\varepsilon > 0$ a coupled linear first-order transport PDE, with terms of orders $O\left(\frac{1}{\varepsilon}\right)$, $O\left(\frac{1}{\varepsilon^2}\right)$ and study under appropriate hypotheses the limit of $\mathbf{w}^\varepsilon$ as $\varepsilon \to 0$. This will be a *diffusion limit*, a sort of twin of the hydrodynamical limit from §V.B.5.

1. Formulation

Our PDE system is

$$\mathbf{w}_t^\varepsilon + \frac{1}{\varepsilon} B D\mathbf{w}^\varepsilon = \frac{1}{\varepsilon^2} C\mathbf{w}^\varepsilon \text{ in } \mathbb{R}^n \times (0,\infty). \tag{1}$$

The unknown is

$$\mathbf{w}^\varepsilon : \mathbb{R}^n \times (0,\infty) \to \mathbb{R}^m,\ \mathbf{w}^\varepsilon = (w^{1,\varepsilon}, \dots, w^{m,\varepsilon}).$$

Notation. In (1) we are given the matrix

$$C = ((c_{kl}))_{m\times m}$$

and also

$$B = \text{ diag}(b^1, \dots, b^m),$$

where the *vectors* $\{b^k\}_{k=1}^m$ in $\mathbb{R}^n$ are given, $b^k = (b_1^k, \dots, b_n^k)$. In terms of the components of $\mathbf{w}^\varepsilon$, our system (1) reads:

$$w_t^{k,\varepsilon} + \frac{1}{\varepsilon} b^k \cdot Dw^{k,\varepsilon} = \frac{1}{\varepsilon^2} \sum_{l=1}^m c_{kl} w^{l,\varepsilon} \tag{2}$$

for $k = 1, \dots, m$. □

Remark. We can think of (2) as a variant of the PDE (63) in §V.B.5, where the velocity parameterization variable y is now discrete. Thus (1) is a scalar PDE for $w^\varepsilon = w^\varepsilon(x, y, t)$, $y \in \{1, \dots, m\}$. □

The left hand side of (1) is for each k a linear, constant coefficient transport operator, and the right hand side of (1) represents linear coupling. As $\varepsilon \to 0$, the velocity $\frac{1}{\varepsilon} b^k$ on the left becomes bigger and the coupling $\frac{1}{\varepsilon^2} C$ on the right gets bigger even faster. What happens in the limit?

To answer we introduce some hypotheses, the meaning of which will be revealed only later. Let us first assume:

$$c_{kl} > 0 \text{ if } k \neq l,\ \sum_{l=1}^m c_{kl} = 0. \tag{3}$$

It follows from Perron–Frobenius theory for matrices that there exists a unique vector

$$\pi = (\pi_1, \dots, \pi_m)$$

satisfying

$$\text{(4)} \qquad \begin{cases} \pi_k > 0 \ (k = 1, \dots, m), \ \sum_{k=1}^m \pi_k = 1, \\ \text{and} \\ \sum_{k=1}^m c_{kl}\pi_k = 0. \end{cases}$$

(See for instance Gantmacher [G] for Perron–Frobenius theory, and also look at §VIII.A below.)

We envision π as a probability vector on $\Omega = \{1, \dots, m\}$ and then make the assumption of *average velocity balance*:

$$\text{(5)} \qquad \sum_{k=1}^m \pi_k b^k = 0.$$

2. Construction of diffusion coefficients

Our goal is to prove that for each $k \in \{1, \dots, m\}$, $w^{k,\varepsilon} \to u$ as $\varepsilon \to 0$, u solving a diffusion equation of the form:

$$u_t - \sum_{i,j=1}^n a_{ij} u_{x_i x_j} = 0 \text{ in } \mathbb{R}^n \times (0, \infty).$$

We must construct the matrix $A = ((a_{ij}))$. First, write $\mathbb{1} = (1, \dots, 1) \in \mathbb{R}^m$. Then (2), (3) say

$$\text{(6)} \qquad C\mathbb{1} = 0, \ C^*\pi = 0.$$

Perron–Frobenius theory tells us that the nullspace of C is one-dimensional and so is spanned by $\mathbb{1}$. Likewise π spans the nullspace of C^*. In view of (5), for each $j \in \{1, \dots, n\}$, the vector $b_j = (b_j^1, \dots, b_j^m) \in \mathbb{R}^m$ is perpendicular to the nullspace of C^* and thus lies in the range of C. Consequently there exists a unique vector $d_i \in \mathbb{R}^m$ solving

$$\text{(7)} \qquad Cd_j = -b_j \qquad (j = 1, \dots, n),$$

normalized by our requiring

$$d_j \cdot \mathbb{1} = 0 \qquad (j = 1, \dots, n).$$

We write $d_j = (d_j^1, \ldots, d_j^m)$, and then define the *diffusion coefficients*

$$a^{ij} = \sum_{k=1}^{m} \pi_k b_i^k d_j^k \qquad (1 \le i, j \le n). \tag{8}$$

Lemma *The matrix $A = ((a^{ij}))$ is nonnegative definite; that is,*

$$\sum_{i,j=1}^{n} a^{ij} \xi_i \xi_j \ge 0 \text{ for each } \xi \in \mathbb{R}^n. \tag{9}$$

Proof. Take $\xi = (\xi_1, \ldots, \xi_n) \in \mathbb{R}^n$ and write

$$\eta_k := \sum_{j=1}^{n} d_j^k \xi_j \qquad (k = 1, \ldots, m).$$

Observe further that (7) says

$$b_i^k = -\sum_{l=1}^{m} c_{kl} d_i^l \qquad (1 \le k \le m,\ 1 \le i \le n). \tag{10}$$

Consequently (8) implies

$$\begin{aligned} \textstyle\sum_{i,j}^{n} a^{ij} \xi_i \xi_j &= -\textstyle\sum_{i,j=1}^{n} \sum_{k,l=1}^{m} \pi_k c_{kl} d_i^l \xi_i d_j^k \xi_j \\ &= -\textstyle\sum_{k,l=1}^{m} \pi_k c_{kl} \eta_l \eta_k \\ &= -\textstyle\sum_{k,l=1}^{m} s_{kl} \eta_k \eta_l, \end{aligned} \tag{11}$$

for

$$s_{kl} := \frac{\pi_k c_{kl} + \pi_l c_{lk}}{2} \qquad (1 \le k, l \le m).$$

The matrix $S = ((s_{kl}))_{m \times m}$ is symmetric, with $s_{kl} > 0$ $(k \ne l)$ and

$$S\mathbb{1} = 0$$

owing to (5). Since obviously the entries of $\mathbb{1} = (1, \ldots, 1)$ are positive, Perron–Frobenius theory asserts that every other eigenvalue of S has real part less than or equal to the eigenvalue (namely 0) associated with $\mathbb{1}$. But as S is symmetric, each eigenvalue is real. So

$$\lambda \le 0$$

for each eigenvalue of S. Consequently (10) follows from (11). □

3. Passage to limits

Assume now

$$g : \mathbb{R}^n \to \mathbb{R}$$

is smooth, with compact support. We introduce the initial value problem for (1):

$$\text{(12)} \qquad \begin{cases} w_t^{k,\varepsilon} + \frac{1}{\varepsilon} b^k \cdot Dw^{k,\varepsilon} = \frac{1}{\varepsilon^2} \sum_{l=1}^m c_{kl} w^{l,\varepsilon} & \text{in } \mathbb{R}^n \times (0,\infty) \\ w^{k,\varepsilon} = g & \text{on } \mathbb{R}^n \times \{t=0\} \end{cases}$$

for $k = 1, \dots, n$. Linear PDE theory implies there exists a unique smooth solution $\mathbf{w}^\varepsilon$.

Theorem *As $\varepsilon \to 0$, we have for $k = 1, \dots, m$:*

$$\text{(13)} \qquad w^{k,\varepsilon} \to u \text{ locally uniformly in } \mathbb{R}^n \times [0,\infty)$$

where u is the unique solution of

$$\text{(14)} \qquad \begin{cases} u_t - \sum_{i,j=1}^n a^{ij} u_{x_i x_j} = 0 \text{ in } \mathbb{R}^n \times (0,\infty) \\ u = g \text{ on } \mathbb{R}^n \times \{t=0\}. \end{cases}$$

Remark. We are asserting that each component $w^{k,\varepsilon}$ of $\mathbf{w}^\varepsilon$ converges to the same limit function $u : \mathbb{R}^n \times [0,\infty) \to \mathbb{R}$ and that u solves the diffusion equation (14).

Proof. 1. See [E2] for a proof that

$$\begin{cases} \{\mathbf{w}^\varepsilon\}_{0<\varepsilon\le 1} \text{ is bounded, uniformly continuous} \\ \text{on compact subsets of } \mathbb{R}^n \times [0,\infty). \end{cases}$$

Thus we can find a subsequence $\varepsilon_r \to 0$ such that

$$\mathbf{w}^{\varepsilon_r} \to \mathbf{w} \text{ locally uniformly,}$$
$$\mathbf{w} = (w^1, \dots, w^m).$$

2. We first *claim* that

$$\text{(15)} \qquad w^1 = w^2 = \cdots = w^m$$

at each point $x \in \mathbb{R}^n$, $t \ge 0$, or—in other words—

$$\mathbf{w} = u\mathbb{1}$$

for some scalar function $u = u(x,t)$. To verify this, take any $\mathbf{v} \in C_c^\infty(\mathbb{R}^n \times (0,\infty);\ \mathbb{R}^m)$ and observe from (11) that

$$\int_0^\infty \int_{\mathbb{R}^n} \mathbf{v} \cdot (C\mathbf{w}^\varepsilon) dxdt = O(\varepsilon).$$

It follows that

$$\int_0^\infty \int_{\mathbb{R}^n} \mathbf{v} \cdot (C\mathbf{w}) dxdt = 0$$

for all $\mathbf{v}$ as above and so $C\mathbf{w} \equiv 0$ in $\mathbb{R}^n \times (0,\infty)$. Since the nullspace of C is the span of $\mathbb{1}$, (14) follows.

3. Thus

$$w^{k,\varepsilon_r} \to u \text{ locally uniformly } (k = 1, \dots, m). \tag{16}$$

We next claim that

$$u \text{ is a viscosity solution of (14).} \tag{17}$$

This means that if $v \in C^2(\mathbb{R}^n \times (0,\infty))$ and

$$\begin{cases} u - v \text{ has a local maximum (resp. minimum) at} \\ \text{a point } (x_0, t_0) \in \mathbb{R}^n \times (0,\infty), \end{cases} \tag{18}$$

Then

$$v_t(x_0,t_0) - \sum_{i,j=1}^n a^{ij} v_{x_i x_j}(x_0,t_0) \le 0 \text{ (resp. } \ge 0). \tag{19}$$

4. To prove this, let us take v as above and suppose $u - v$ has a *strict* local maximum at some point (x_0, t_0). Define then the *perturbed test functions*

$$\mathbf{v}^\varepsilon := (v^{1,\varepsilon}, \dots, v^{m,\varepsilon}),$$

where

$$v^{k,\varepsilon} := v - \varepsilon \sum_{j=1}^n d_j^k v_{x_j} \qquad (k = 1, \dots, m), \tag{20}$$

the constants d_j^k $(1 \le j \le n,\ 1 \le k \le m)$ satisfying (7). Clearly

$$v^{k,\varepsilon_r} \to v \text{ locally uniformly } (k = 1, \dots, m). \tag{21}$$

Since $u - v$ has a strict local maximum at (x_0, t_0), it follows from (16), (21) that

$$\text{(22)} \qquad \begin{cases} w^{k,\varepsilon} - v^{k,\varepsilon} \text{ has a local maximum near } (x_0, t_0) \\ \text{at a point } (x_\varepsilon^k, t_\varepsilon^k) \ (k = 1, \dots, m), \end{cases}$$

for $\varepsilon = \varepsilon_r$, and

$$\text{(23)} \qquad (x_\varepsilon^k, t_\varepsilon^k) \to (x_0, t_0) \text{ as } \varepsilon = \varepsilon_r \to 0, \ k = 1, \dots, m.$$

Since $\mathbf{w}^\varepsilon$ and $\mathbf{v}^\varepsilon$ are smooth functions, it follows from (22) and the PDE (12) that:

$$\text{(24)} \qquad v_t^{k,\varepsilon} + \frac{1}{\varepsilon} b^k \cdot Dv^{k,\varepsilon} = \frac{1}{\varepsilon^2} \sum_{l=1}^m c_{kl} w^{\varepsilon,l}$$

at the point $(x_\varepsilon^k, t_\varepsilon^k)$, $\varepsilon = \varepsilon_r$. Recalling (20), we conclude from (24) that

$$\text{(25)} \qquad \begin{array}{rcl} v_t(x_0, t_0) & - & \sum_{i,j=1}^n b_i^k d_j^k v_{x_i x_j}(x_0, t_0) \\ & = & -\frac{1}{\varepsilon} \sum_{i=1}^n b_i^k v_{x_i}(x_\varepsilon^k, t_\varepsilon^k) \\ & + & \frac{1}{\varepsilon^2} \sum_{l=1}^m c_{kl} w^{\varepsilon,l}(x_\varepsilon^k, t_\varepsilon^k) + o(1) \end{array}$$

as $\varepsilon = \varepsilon_r \to 0$, $k = 1, \dots, m$.

5. Now since $w^{\varepsilon,l} - v^{\varepsilon,l}$ has its local maximum near (x_0, t_0) at $(x_\varepsilon^l, t_\varepsilon^l)$, we have

$$\text{(26)} \qquad (w^{\varepsilon,l} - v^{\varepsilon,l})(x_\varepsilon^l, t_\varepsilon^l) \geq (w^{\varepsilon,l} - v^{\varepsilon,l})(x_\varepsilon^k, t_\varepsilon^k),$$

$\varepsilon = \varepsilon_r$. Recalling that $c_{kl} > 0$ for $k \neq l$, we can employ the inequalities (26) in (25):

$$\begin{array}{rcl} v_t(x_0, t_0) & - & \sum_{i,j=1}^n b_i^k d_j^k v_{x_i x_j}(x_0, t_0) \\ & \leq & -\frac{1}{\varepsilon} \sum_{i=1}^n b_i^k v_{x_i}(x_\varepsilon^k, t_\varepsilon^k) \\ & + & \frac{1}{\varepsilon^2} \sum_{l=1}^m c_{kl} \left[(w^{\varepsilon,l} - v^{\varepsilon,l})(x_\varepsilon^l, t_\varepsilon^l) + v(x_\varepsilon^k, t_\varepsilon^k) - \varepsilon \sum_{i=1}^n d_i^l v_{x_i}(x_\varepsilon^k, t_\varepsilon^k) \right] \\ & + & o(1). \end{array}$$

But (10) says $\sum_{l=1}^m c_{kl} d_i^l = -b_i^k$, and so the $O\left(\frac{1}{\varepsilon}\right)$ terms in the foregoing expression cancel out. Thus

$$\begin{array}{rcl} v_t(x_0, t_0) & - & \sum_{i,j=1}^n b_i^k d_j^k v_{x_i x_j}(x_0, t_0) \\ & \leq & \frac{1}{\varepsilon^2} \sum_{l=1}^m c_{kl} [(w^{\varepsilon,l} - v^{\varepsilon,l})(x_\varepsilon^l, t_\varepsilon^l) + v(x_\varepsilon^k, t_\varepsilon^k)]. \end{array}$$

Multiply by $\pi_k > 0$ and sum $k = 1, \dots, m$, recalling (2), (3) to deduce:

$$\begin{array}{rcl} v_t(x_0, t_0) & - & \sum_{i,j=1}^n \underbrace{\left(\sum_{k=1}^n \pi_k b_i^k d_j^k \right)}_{a^{ij}} v_{x_i x_j}(x_0, t_0) \\ & \leq & o(1). \end{array}$$

Let $\varepsilon = \varepsilon_r \to 0$ to derive the inequality (19). A simple approximation removes the requirement at $u - v$ have a strict maximum, and a similar argument derives the opposite inequality should $u - v$ have a minimum at (x_0, t_0). □

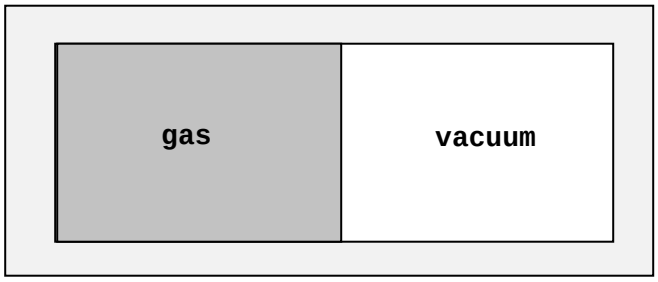
Commentary. The linear system (12) for each fixed $\varepsilon > 0$ represents a system of linear transport PDE with simple linear coupling. This PDE is reversible in time and yet the diffusion equation (14) is not. The interesting question is this: *where did the irreversibility come from*? Section VIII.A will provide some further insights. See also Pinsky [P] for other techniques, mostly based upon interpreting (12) as a *random evolution*. □

CHAPTER 7: Entropy and uncertainty

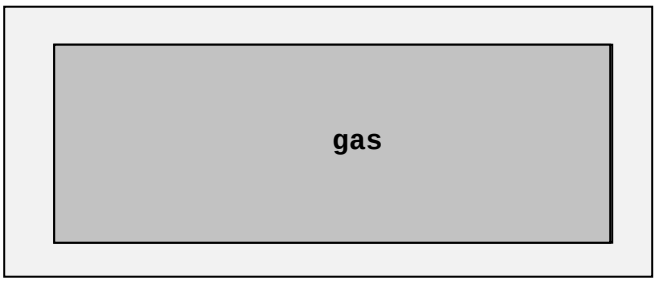
In this and the subsequent chapter we consider various *probabilistic* aspects of entropy and some implications for PDE theory. The present chapter is a quick introduction to entropy in statistical mechanics.

A. Maxwell's demon

Let us begin with a simple physical situation, consideration of which will soon suggest that there is some kind of connection between entropy, information, and uncertainty.



initial state



final state

Take one mole of a simple ideal gas, and suppose it is initially at equilibrium, being held by a partition in half of a thermally insulated cylinder. The initial volume is V_i, and the initial temperature is T_i. We remove the partition, the gas fills the entire cylinder, and, after coming to equilibrium, it has final volume V_f, final temperature T_f.

What is the change of entropy? According to §I.F, we have

$$\text{(1)} \qquad \begin{cases} S_i &= C_V \log T_i + R \log V_i + S_0 \\ S_f &= C_V \log T_f + R \log V_f + S_0, \end{cases}$$

so being an arbitrary constant. As there is no heat transfer nor work done to or from the exterior, the internal energy is unchanged. Since, furthermore, the energy depends only on the temperature (see §I.F), we deduce

$$T_i = T_f.$$

As $V_f = 2V_i$, we deduce that the change of entropy is

$$S_f - S_i = R \log 2 > 0,$$

in accordance with the Second Law. The mole of gas contains N_A molecules, and so

$$\text{change of entropy/particle } = k \log 2, \tag{2}$$

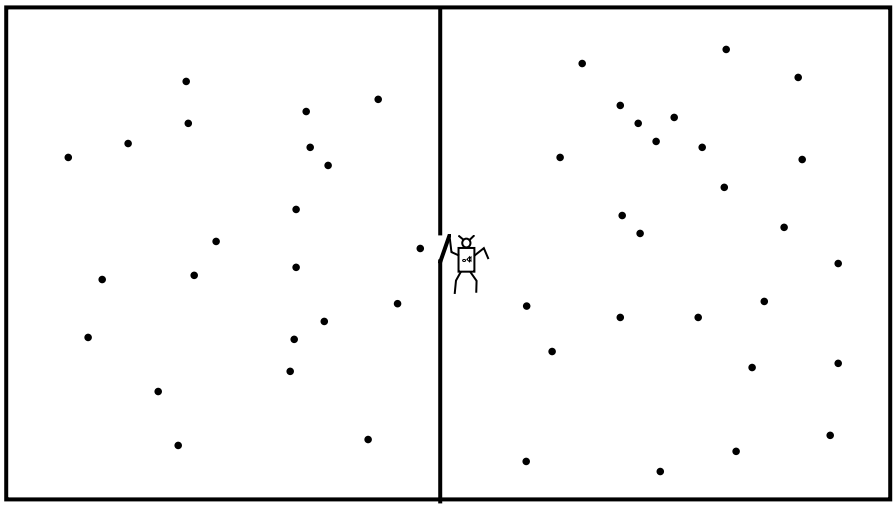
since $k = R/N_A$.

As the last sentence suggests, it is convenient now to shift attention to the microscopic level, at which the gas can be thought of as a highly complex, random motion of N_A molecules. We next imagine that we reinstall the partition, but now with

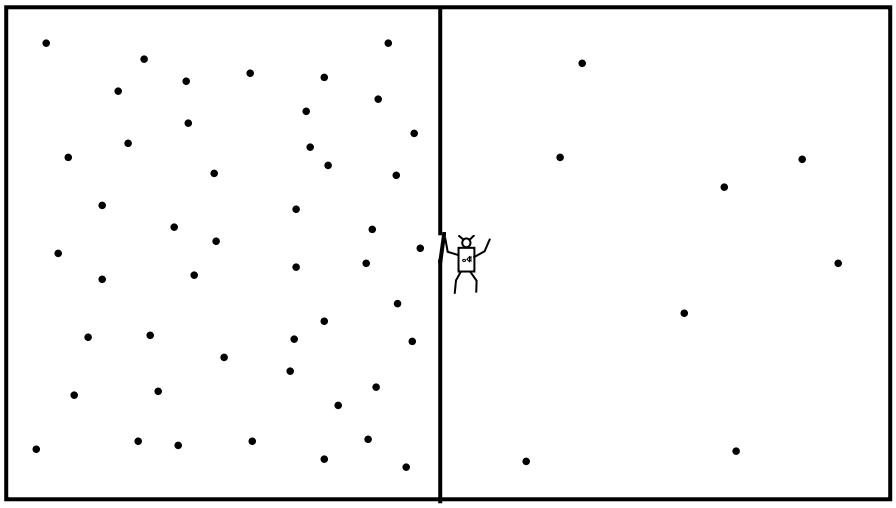
(a) a small gate

and

(b) a nanotechnology-built robot, which acts as a gatekeeper.



Our robot is programmed to open the door whenever a gas molecule approaches the door from the right, but to close the door if a gas molecule approaches from the left. After our robot has been at work for awhile, we will see more particles in the left region than in the right. This is close to our initial situation.



The effect of our tiny robot has thus been to *decrease* the entropy, with a very small expenditure of energy on its part. We have here an apparent contradiction of the Second Law.

Maxwell in 1867 proposed this thought experiment, with an intelligent creature (called "Maxwell's demon" by Kelvin) in place of our nanoscale robot. Generations of physicists have reconsidered this problem, most notably L. Szilard [SZ], who argued that the Second Law is not violated provided the overall entropy of the system *increases* by $k \log 2$ each time the robot measures the direction of an incoming molecule in order to decide whether or not to open the gate. As (2) presumably implies the entropy *decreases* by $k \log 2$ once a particle is trapped on the left, the Second Law is saved, provided—to repeat—we appropriately assign an entropy to the robot's gaining information about molecule velocities.

We will not attempt to pursue such reasoning any further, being content to learn from this thought experiment that there seems to be some sort of connection between entropy and our information about random systems.

Remark. The book [L-R], edited by Leff and Rex, is a wonderful source for more on Maxwell's demon, entropy concepts in computer science, etc. See also the website `www.math.washington.edu/~hillman/entropy.html`. □

B. Maximum entropy

This section introduces a random model for thermal systems and a concept of entropy as a measure of uncertainty. The following is based upon Huang [HU], Jaynes [J], Bamberg–Sternberg [B-S].

1. A probabilistic model

A probabilistic model for thermal systems in equilibrium

We are given:

(i) a triple

$$(\Omega, \mathcal{F}, \pi),$$

consisting of a set Ω, a σ-algebra $\mathcal{F}$ of subsets of Ω, and a nonnegative measure π defined on $\mathcal{F}$. (We call $(\Omega, \mathcal{F}, \pi)$ the *system*, and π the reference *measure*. A typical point $\omega \in \Omega$ is a *microstate*.)

(ii) the collection of all π-measurable functions

$$\rho : \Omega \to [0, \infty),$$

such that

$$\int_\Omega \rho d\pi = 1. \tag{1}$$

(We call such a ρ the *density* of the *microstate measure* $\rho d\pi$)

and

(iii) a π-measurable function

$$\mathbf{X} : \Omega \to \mathbb{R}^{m+1},\ \mathbf{X} = (X^0, \ldots, X^m). \tag{2}$$

(We call each X^k an *observable*.)

Notation.

$$\begin{array}{rcl} E(\mathbf{X}, \rho) & = & \langle \mathbf{X} \rangle = \int_\Omega \mathbf{X} \rho d\pi \\ & = & \textit{expected value} \text{ of } \mathbf{X}, \text{ given the} \\ & & \text{microstate distribution } \rho. \end{array} \tag{3}$$

□

Physical interpretation. We think of Ω as consisting of a huge number of microstates ω, each of which is equivalent to a precise, detailed microscopic description of some physical system, e.g. an exact description of the behavior of all the particles in a mole of gas.

The main point is that Ω *is not observable physically.* We instead model the state of the system by the probability measure

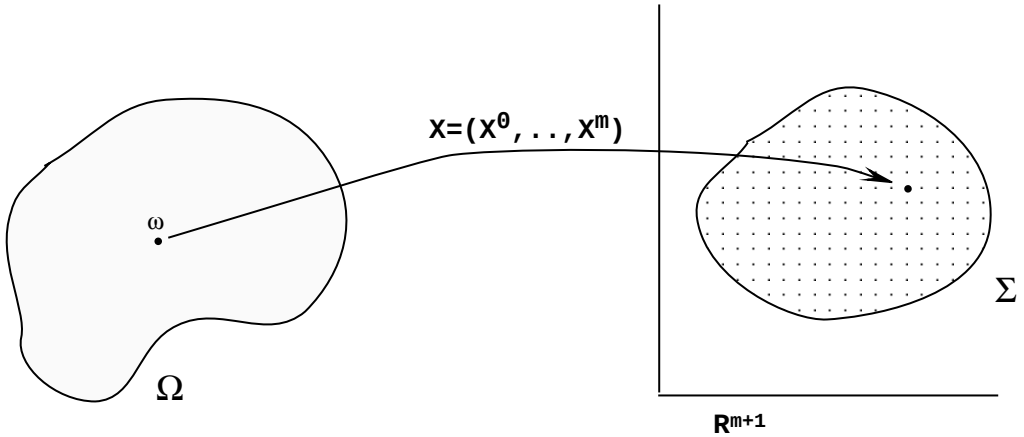
$$\rho d\pi,$$

where ρ satisfies (1). Thus if $E \in \mathcal{F}$, then

$$\int_E \rho d\pi$$

is the probability that the true (but unobserved) microstate is in E, given the density ρ. Our goal is to determine, or more precisely to estimate ρ, given certain *macroscopic* physical measurements.

These we model using the observables $X^0, \ldots, X^m$.



Given ρ as above, we assume that we can physically measure the values

$$E(\mathbf{X}, \rho) = \langle \mathbf{X} \rangle = \bar{X}. \tag{4}$$

Think of the point $\bar{X} = (\bar{X}_0, \ldots, \bar{X}_m)$ as lying in some region $\Sigma \subset \mathbb{R}^{m+1}$, which we may interpret as the *macroscopic state space*. A point $\bar{X} \in \Sigma$ thus corresponds to $m+1$ physical measurements, presumably of extensive parameters as in Chapter I. To accord with the notation from §I.A, we will often write

$$E = \langle X^0 \rangle. \tag{5}$$

□

The fundamental problem is this. Given the macroscopic measurements $\bar{X} = (\bar{X}_0, \bar{X}_1, \ldots, \bar{X}_m)$, there are generally many, many microstate distributions ρ satisfying (4). How do we determine the "physically correct" distribution?

2. Uncertainty

To answer the question just posed, let us first consider the special case that

$$\begin{cases} \Omega = \{\omega_1, \ldots, \omega_N\} \text{ is a finite set, } \mathcal{F} = 2^\Omega, \\ \text{and } \pi \text{ is counting measure.} \end{cases} \tag{6}$$

Then each distribution ρ as above corresponds to our assigning $\rho(\omega_i) = p_i$ $(i = 1, \ldots, N)$, where

$$0 \leq p_i \leq 1 \ (i = 1, \ldots, N), \ \sum_{i=1}^{N} p_i = 1 \tag{7}$$

Thus p_i is the probability of ω_i.

We propose now to find a function $S = S(p_1, \ldots, p_N)$ which somehow measures the *uncertainty* or *disorder* inherent in the probability distribution $\{p_1, \ldots, p_N\}$. Let us imagine S is defined for all $N = 1, 2, \ldots$ and all N-tuples $\{p_1, \ldots, p_N\}$ as above.

We will ordain these

Axioms for S:

A. Continuity

For each N, the mapping $(p_1, \ldots, p_N) \mapsto S(p_1, \ldots, p_N)$ is continuous.

B. Monotonicity

The mapping $N \mapsto S\left(\frac{1}{N}, \ldots, \frac{1}{N}\right)$ is monotonically increasing.

C. Composition

For each N and each probability distribution $(p_1, \ldots, p_N)$, set

$$q_1 = p_1 + \cdots + p_{k_1}, \ldots, q_j = p_{k_{j-1}+1} + \cdots + p_{k_j}, \ldots$$

where $1 = k_0 \leq k_1 \leq k_2 \leq \cdots \leq k_M = N$. Then

$$\begin{cases} S(p_1, \ldots, p_N) & = & S(q_1, \ldots, q_M) \\ & + & \sum_{j=1}^{M} q_j S(p_{k_{j-1}+1}/q_j, \ldots, p_{k_j}/q_j). \end{cases} \tag{8}$$

Probabilistic interpretation

The monotonicity rule B says that if all the points in $\Omega = \{\omega_1, \ldots, \omega_N\}$ have equal probability $\frac{1}{N}$, then there is more uncertainty the bigger N is. The composition rule C applies if we think of subdividing $\Omega = \bigcup_{i=1}^{M} \Omega_j$, where $\Omega_j = \{\omega_{k_{j-1}+1}, \ldots, \omega_{k_j}\}$. Then q_j is the probability of the event Ω_j. Further (8) says that the uncertainty inherent in the distribution $\{p_1, \ldots, p_N\}$ on Ω should equal the uncertainty of the induced probability distribution $\{q_1, \ldots, q_M\}$ on $\{\Omega_1, \ldots, \Omega_M\}$ *plus* the "average of the uncertainties within each Ω_j". This last expression is the sum on j of q_j, the probability of Ω_j, times S computed for the induced probability distribution $\{p_{k_{j-1}+1}/q_j, \ldots, p_{k_j}/q_j\}$ on Ω_j. If some $q_j = 0$, we omit this term. □

Lemma. *The axioms imply S has the form*

$$S(p_1, \ldots, p_N) = -K \sum_{i=1}^{N} p_i \log p_i \tag{9}$$

for some positive constant K.

Proof. 1. We follow Jaynes [J]. Suppose S satisfies Axioms A–C, and define

$$A(N) := S\left(\underbrace{\frac{1}{N}, \ldots, \frac{1}{N}}_{N \text{ terms}}\right). \tag{10}$$

Take

$$p_i = \frac{1}{N} \qquad (i = 1, \ldots, N),$$

and

$$q_j = \frac{n_j}{N} \qquad (j = 1, \ldots, M), \tag{11}$$

where $\{n_j\}_{j=1}^{M}$ are integers satisfying

$$\sum_{j=1}^{M} n_j = N. \tag{12}$$

Then (8) implies

$$S\left(\frac{1}{N}, \ldots, \frac{1}{N}\right) = S(q_1, \ldots, q_M) + \sum_{j=1}^{M} q_j S\left(\frac{1}{n_j}, \ldots, \frac{1}{n_j}\right).$$

In terms of (10), this equality reads

$$A(N) = S(q_1, \ldots, q_M) + \sum_{j=1}^{M} q_j A(n_j). \tag{13}$$

Now select N of the form

$$N = ML,$$

and set $n_j = L$ for $j = 1, \ldots, M$. Then (13) implies

$$\begin{aligned} A(ML) &= S\left(\tfrac{1}{M}, \ldots, \tfrac{1}{M}\right) + \textstyle\sum_{j=1}^{M} \tfrac{1}{M} S\left(\tfrac{1}{L}, \ldots, \tfrac{1}{L}\right) \\ &= A(M) + A(L). \end{aligned}$$

Thus in particular

$$A(N^a) = aA(N) \text{ for positive integers } a, N. \tag{14}$$

Axiom B implies then $A(N) > 0$ $(N = 2, \dots)$.

2. We claim that in fact

$$\begin{cases} A(N) = K \log N \ (N = 1, \dots) \\ \text{for some positive constant } K. \end{cases} \tag{15}$$

To prove this, let M, N be any integers greater than one. Given any large integer a_k, choose the integer b_k so that

$$M^{b_k} \le N^{a_k} \le M^{b_{k+1}}. \tag{16}$$

Then

$$b_k \log M \le a_k \log N \le (b_k + 1) \log M,$$

and so

$$\frac{\log M}{\log N} \le \frac{a_k}{b_k} \le \left(1 + \frac{1}{b_k}\right) \frac{\log M}{\log N}. \tag{17}$$

Now since $N \mapsto A(N)$ is increasing according to Axiom B, (16) and (14) imply

$$b_k A(M) \le a_k A(N) \le (b_k + 1) A(M).$$

Then, since $A(M) > 0$,

$$\frac{b_k}{a_k} \le \frac{A(N)}{A(M)} \le \frac{b_k + 1}{a_k}. \tag{18}$$

Sending a_k and thus $b_k \to \infty$, we conclude from (17), (18) that

$$\frac{A(N)}{A(M)} = \frac{\log N}{\log M} \qquad (M, N \ge 2).$$

This identity implies $A(N) = K \log N$ for some constant K, and necessarily $K > 0$ in light of Axiom B. This proves (15).

3. Now drop the assumption that $n_j = L$ $(j = 1, \dots, M)$. We then deduce from (11)–(15) that

$$\begin{aligned} S\left(\tfrac{n_1}{N}, \dots, \tfrac{n_M}{N}\right) &= A(N) - \textstyle\sum_{j=1}^{M} \frac{n_j}{N} A(n_j) \\ &= K\left(\log N - \textstyle\sum_{j=1}^{M} \frac{n_j}{N} \log n_j\right) \\ &= -K \textstyle\sum_{j=1}^{M} \frac{n_j}{N} \log\left(\frac{n_j}{N}\right) \end{aligned}$$

provided $n_1, \ldots, n_M$ are nonnegative integers summing to N. In view of Axiom A, formula (9) follows. □

We henceforth agree to take $K = k$, Boltzmann's constant, this choice being suggested by the physical calculations in §V.A.2. Thus

$$S(p_1, \ldots, p_N) = -k \sum_{i=1}^{N} p_i \log p_i$$

provided $0 \leq p_i \leq 1$ $(i = 1, \ldots, N)$, $\sum_{i=1}^{N} p_i = 1$.

Return now to the general probabilistic model in §1 for a thermal system in equilibrium. Motivated both by the above formula and our earlier study of Boltzmann's equation in V.A.2, we hereafter define

$$S(\rho) = -k \int_\Omega \rho \log \rho d\pi \tag{19}$$

to be the *entropy* of the microstate density ρ, *with respect to the reference measure* π. We interpret $S(\rho)$ as measuring the uncertainty or disorder inherent in the probability distribution $\rho d\pi$.

C. Maximizing uncertainty

We can now provide an answer to the question posed at the end of §1, namely how to select the "physically correct" microstate distribution satisfying the macroscopic constraints

$$E(X^k, \rho) = \bar{X}_k \qquad (k = 0, \ldots, m)? \tag{20}$$

Here is the idea: Since all we really know about ρ are these identities,

$$\left\{ \begin{array}{l} \textit{we should select the distribution } \rho \textit{ which maximizes} \\ \textit{the uncertainty (= entropy) } S(\rho), \textit{ subject to the} \\ \textit{constraints } (20). \end{array} \right.$$

Remark. This is both a principle of physics (that we should seek maximum entropy configurations (§I.C.6)) and a principle of statistics (that we must employ unbiased estimators). See Jaynes [J] for a discussion of the latter. □

We analyze the foregoing entropy maximization principle by introducing the admissible class:

$$\mathcal{A} = \left\{ \rho : \Omega \to [0, \infty) \mid \rho \text{ is } \pi\text{-measurable}, \ \int_\Omega \rho d\pi = 1, \ E(\mathbf{X}, \rho) = \bar{X} \right\}, \tag{21}$$

where $\bar{X} = (\bar{X}_0, \ldots, \bar{X}_m)$ is given. Recall that we write $\mathbf{X} : \Omega \to \mathbb{R}^{m+1}$, $\mathbf{X} = (X^0, \ldots, X^m)$.

Theorem. (i) *Assume there exist* $\beta \in \mathbb{R}^{m+1}$ *and* $Z > 0$ *such that*

$$\sigma = \frac{e^{-\beta \cdot \mathbf{X}}}{Z} \tag{22}$$

belongs to $\mathcal{A}$. *Then*

$$S(\sigma) = \max_{\rho \in \mathcal{A}} S(\rho). \tag{23}$$

(ii) *Any other maximizer of* $S(\cdot)$ *over* $\mathcal{A}$ *differs from* σ *only on a set of* π*-measure zero.*

Remark. Observe

$$Z = \int_\Omega e^{-\beta \cdot \mathbf{X}} d\pi. \tag{24}$$

□

Proof. 1. First note that

$$\psi(x) := \frac{1}{x} + \log x \qquad (x > 0)$$

satisfies

$$\psi'(x) = -\frac{1}{x^2} + \frac{1}{x} \begin{cases} > 0 & \text{if } x \geq 1 \\ < 0 & \text{if } 0 < x \leq 1. \end{cases}$$

Hence

$$\psi(x) \geq \psi(1) = 1 \text{ for all } x > 0,$$

and so

$$\phi(x) := x \log x - x + 1 \geq 0 \qquad (x > 0), \tag{25}$$

with equality only for $x = 1$.

2. Define σ by (20) and take $\rho \in \mathcal{A}$. Then

$$-\rho \log \rho + \rho \log \sigma \leq \sigma - \rho \text{ on } \Omega, \tag{26}$$

since this inequality is equivalent to

$$\frac{\rho}{\sigma} \log \left(\frac{\rho}{\sigma} \right) - \frac{\rho}{\sigma} + 1 = \phi \left(\frac{\rho}{\sigma} \right) \geq 0.$$

In view of (25) then, (26) holds.

3. Integrate (26) over Ω:

$$-\int_\Omega \rho \log \rho d\pi \leq -\int_\Omega \rho \log \sigma d\pi. \tag{27}$$

But in light of (21):

$$\log \sigma = -\log Z - \beta \cdot \mathbf{X},$$

and so

$$\begin{aligned} \int_\Omega \rho \log \sigma d\pi &= -\log Z - \beta \cdot \int_\Omega \rho \mathbf{X} d\pi \\ &= -\log Z - \beta \cdot \bar{X}, \end{aligned}$$

since $\rho \in \mathcal{A}$. Since $\sigma \in \mathcal{A}$ as well,

$$\begin{aligned} \int_\Omega \sigma \log \sigma d\pi &= -\log Z - \beta \cdot \bar{X} \\ &= \int_\Omega \rho \log \sigma d\pi. \end{aligned}$$

Consequently (27) implies

$$S(\rho) \leq S(\sigma). \tag{28}$$

We have a strict inequality here unless we have equality in (26) π–a.e., and this in turn holds only if $\rho = \sigma$ π–a.e. □

D. Statistical mechanics

1. Microcanonical distribution

We consider in somewhat more detail first of all the case that *there are no observables*, in which case we deduce from Theorem 1 in §B that the entropy $S(\cdot)$ is maximized by the constant microstate distribution

$$\sigma \equiv \frac{1}{Z}, \tag{1}$$

where

$$Z = \pi(\Omega). \tag{2}$$

Thus each microstate is equally probable. This is the *microcanonical distribution* (a.k.a. microcanonical ensemble).

Example 1. Let us take Ω to be a finite set,

$$\Omega = \{\omega_1, \ldots, \omega_N\},$$

and take the reference measure π to be counting measure. Then (1), (2) imply $Z = N$, $\sigma(\omega_i) = \frac{1}{N}$ for $i = 1, \ldots, N$. The entropy is

$$\begin{aligned} S(\sigma) &= -k \textstyle\sum_{i=1}^N \sigma(\omega_i) \log(\sigma(\omega_i)) \\ &= k \log N. \end{aligned}$$

This formula is usually written

$$S = k \log W \tag{3}$$

where $W = N = |\Omega|$. □

Example 2. Assume we are given a smooth function

$$H : \mathbb{R}^n \to \mathbb{R},$$

called the *Hamiltonian*. Fix a number $E \in \mathbb{R}$ and set

$$\Omega_E = \{x \in \mathbb{R}^n \mid H(x) = E\}.$$

We assume that Ω_E is a smooth, $(n-1)$-dimensional surface in $\mathbb{R}^n$. Consider now the "energy band" $\Delta_\delta = \{x \in \mathbb{R}^n \mid E - \delta \leq H(x) \leq E + \delta\}$ for small $\delta > 0$ and note

$$|\Delta_\delta| = \int_{E-\delta}^{E+\delta} \left(\int_{\{H=t\}} \frac{dS}{|DH|} \right) dt$$

according to the Coarea Formula. (See [E-G].) It follows that

$$\lim_{\delta \to 0} \frac{|\Delta_\delta|}{2\delta} = \int_{\Omega_E} \frac{dS}{|DH|},$$

assuming Ω_E is a smooth surface and $|DH| > 0$ on Ω_E. Here dS is $(n-1)$-dimensional surface measure. Now take

$$d\pi = \frac{1}{|DH|}\, dS, \quad \Lambda(E) = \int_{\Omega_E} \frac{dS}{|DH|}.$$

The entropy is then

$$\S(E) = k \log \Lambda(E). \tag{4}$$

Physical interpretation. The Hamiltonian gives us the energy of each microstate. We are here assuming our system is *thermally isolated*, so that all attainable microstates lie on the energy surface $\{H = E\}$, where E is the macroscopic energy. We can, as in Chapter I, define the *temperature* T by

$$\frac{1}{T} = \frac{\partial S}{\partial E}.$$

Remark. Notice that our choice $d\pi = \frac{1}{|DH|}\, dS$ depends not only on the geometry of the level set $\{H = E\}$, but also on $|DH|$. Another plausible possibility would therefore be simply to take $d\pi = dS$.

The issue here is to understand the physical differences between taking the "hard" constraint $H = E$ versus the limit as $\delta \to 0$ of the "softer" constraints $E - \delta \leq H \leq E + \delta$.

The expository paper [vK-L] by van Kampen and Lodder discusses this and some related issues. □

2. Canonical distribution

Next we apply the results of §B to the case that we have one observable $X^0 = H$, where

$$H : \Omega \to \mathbb{R}$$

is the Hamiltonian. As before we write E for the macroscopic energy:

$$E = \langle H \rangle. \tag{5}$$

We now invoke Theorem 1 from §B to deduce that the entropy $S(\cdot)$ is maximized by the microstate distribution

$$\sigma = \frac{e^{-\beta H}}{Z} \text{ for some } \beta \in \mathbb{R}, \tag{6}$$

where

$$Z = \int_\Omega e^{-\beta H} d\pi. \tag{7}$$

This is the *canonical distribution* (a.k.a. Gibbs' distribution, canonical ensemble). We assume the integral in (7) converges.

Physical interpretation. We should in this context imagine our system as not being thermally isolated, but rather as being in thermal contact with a "heat reservoir" and so being held at a constant temperature T. In this setting energy can be transferred in and out of our system. Thus the energy level H of the various microstates is not constant (as in Example 2 in §1) but rather its average value $\langle H \rangle = E$ is determined, as we will see, by T. □

Example. Let us take $\Omega = \mathbb{R}^3$, π to be Lebesgue measure, and

$$H = \frac{m}{2}|v|^2 \qquad (v \in \mathbb{R}^3).$$

H is the kinetic energy of a particle with mass $m > 0$, velocity v. Then canonical distribution is then

$$\sigma = \frac{1}{Z} e^{-\beta \frac{m|v|^2}{2}}.$$

But this is essentially the Boltzmann distribution (43) from §V.A.2, with the macroscopic velocity $\mathbf{v} = 0$, the macroscopic particle density $n = 1$, and

$$\beta = \frac{1}{k\theta},$$

θ being the temperature. □

3. Thermodynamics

We next show how to recover aspects of classical equilibrium thermodynamics (as in Chapter I) from the canonical distribution (6), (7). The point is that all the relevant information is encoded within

$$Z = \int_\Omega e^{-\beta H} d\pi. \tag{8}$$

We regard (8) as a formula for Z as a function of β and call Z the *partition function*. Remember $H : \Omega \to \mathbb{R}$.

Definitions of thermodynamic quantities in terms of β and Z. We define

(i) the *temperature* T by the formula

$$\beta = \frac{1}{kT}, \tag{9}$$

(ii) the *energy*

$$E = -\frac{\partial}{\partial \beta}(\log Z), \tag{10}$$

(iii) the *entropy*

$$S = k(\beta E + logZ), \tag{11}$$

and

(iv) the *free energy*

$$F = -\frac{1}{\beta} \log Z. \tag{12}$$

Note carefully: we regard (10)–(12) as defining E, S, F as functions of β.

We must check that these definitions are consistent with everything before:

Theorem. (i) *We have*

$$E = \langle H \rangle, \tag{13}$$

the expected value of H being computed with respect to the canonical distribution $\sigma = \frac{1}{Z} e^{-\beta H}$.

(ii) *Furthermore*

$$S = S(\sigma) = -k \int_\Omega \sigma \log \sigma d\pi, \tag{14}$$

and

$$\frac{\partial S}{\partial E} = \frac{1}{T}. \tag{15}$$

(iii) *Finally,*

$$F = E - ST \tag{16}$$

and

$$\frac{\partial F}{\partial T} = -S. \tag{17}$$

Proof. 1. Using the definition (10) we calculate

$$\begin{aligned} E = -\tfrac{1}{Z}\tfrac{\partial Z}{\partial \beta} &= \tfrac{1}{Z}\textstyle\int_\Omega H e^{-\beta H} d\pi \\ &= \textstyle\int_\Omega H \sigma d\pi = \langle H \rangle. \end{aligned}$$

This is assertion (i) of the Theorem.

2. We compute as well

$$\begin{aligned} S(\sigma) &= -k \textstyle\int_\Omega \sigma \log \sigma d\pi \\ &= -\tfrac{k}{Z} \textstyle\int_\Omega e^{-\beta H}(-\beta H - \log Z) d\pi \\ &= k\beta E + k \log Z. \end{aligned}$$

From (11) we conclude that the identity (14) is valid. Furthermore

$$\begin{aligned} \tfrac{\partial S}{\partial E} &= \tfrac{\partial S}{\partial \beta} \left(\tfrac{\partial E}{\partial \beta} \right)^{-1} \\ &= k \left(E + \beta \tfrac{\partial E}{\partial \beta} + \tfrac{\partial}{\partial \beta}(\log Z) \right) \left(\tfrac{\partial E}{\partial \beta} \right)^{-1} \\ &= k\beta \text{ by (10)} \\ &= \tfrac{1}{T} \text{ by (9)}. \end{aligned}$$

3. Since (12) says $\log Z = -\beta F$, formulas (9), (11) imply $F = E - TS$. This is (16). We next rewrite (12) to read:

$$\int_\Omega e^{-\beta H} d\pi = e^{-\beta F} \tag{18}$$

and so

$$\int_\Omega e^{\beta(F-H)} d\pi = 1.$$

Differentiate with respect to β, recalling that F is a function of β:

$$\int_\Omega \left(F - H + \beta \frac{\partial F}{\partial \beta} \right) e^{\beta(F-H)} d\pi = 0.$$

Thus (13), (18) imply

$$F - E + \beta \frac{\partial F}{\partial \beta} = 0. \tag{19}$$

Now since $\beta = \frac{1}{kT}$,

$$\frac{\partial}{\partial \beta} = -\frac{1}{k\beta^2} \frac{\partial}{\partial T}. \tag{20}$$

Therefore

$$\beta \frac{\partial F}{\partial \beta} = -\frac{1}{k\beta} \frac{\partial F}{\partial T} = -T \frac{\partial F}{\partial T}.$$

Then (19) says

$$F = E + T \frac{\partial F}{\partial T}.$$

Owing to formula (16), we deduce $S = -\frac{\partial F}{\partial T}$. □

Remark. We can define as well the *heat capacity*

$$C_V = k\beta^2 \frac{\partial^2}{\partial \beta^2} (\log Z). \tag{21}$$

Thus (10), (20) say

$$C_V = \frac{\partial E}{\partial T}, \tag{22}$$

consistently with classical thermodynamics. Now since

$$E = \langle H \rangle = \frac{1}{Z} \int_\Omega H e^{-\beta H} d\pi = \int_\Omega H e^{\beta(F-H)} d\pi,$$

we have

$$\int_\Omega (E-H)e^{\beta(F-H)}d\pi = 0.$$

Differentiate with respect to β:

$$\frac{\partial E}{\partial \beta} + \int_\Omega (E-H)\left(F - H + \beta\frac{\partial F}{\partial \beta}\right)e^{\beta(F-H)}d\pi = 0.$$

But $F + \beta\frac{\partial F}{\partial \beta} = E - TS - \frac{1}{k\beta}\frac{\partial F}{\partial T} = E$ and so

$$\langle E-H\rangle^2 = -\frac{\partial E}{\partial \beta} = \frac{\partial^2}{\partial \beta^2}(\log Z).$$

Rewriting, we obtain the formula

$$\langle E-H\rangle^2 = kT^2 C_V, \tag{23}$$

the average on the left computed with respect to the canonical density. This is a probabilistic interpretation of the heat capacity, recording the *variance* of the microstate energy H from its macroscopic mean value $E = \langle H\rangle$. □

Remark. Finally we record the observations that the mapping

$$\beta \mapsto \log Z = \log\left(\int_\Omega e^{-\beta H}d\pi\right) \tag{24}$$

is uniformly convex,

$$S = \min_\beta k(\beta E + \log Z), \tag{25}$$

and

$$\log Z = \max_E \left(-\beta E + \frac{S}{k}\right), \tag{26}$$

where in (25), (26) we regard $S = S(E)$, $Z = Z(\beta)$.

Indeed, we just computed $\frac{\partial^2}{\partial \beta^2}(\log Z) = \langle E-H\rangle^2 > 0$ (unless $H \equiv E$). Consequently the minimum on the right hand side of (25) is attained at the unique β for which

$$\frac{\partial}{\partial \beta}(\log Z) = -E,$$

in accordance with (10). Thus (25) follows from (11). Formula (26) is dual to (25).

Observe that (25), (26) imply:

$$\begin{cases} E \mapsto S \text{ is concave,} \\ \beta \mapsto \log Z \text{ is convex.} \end{cases}$$

□

CHAPTER 8: Probability and PDE

This chapter introduces some further probabilistic viewpoints that employ entropy notions. These in turn give rise in certain settings to various PDE.

A. Continuous time Markov chains

We begin however with a simple system of linear ODE. This example both illustrates how entropy controls convergence to equilibrium for Markov chains and also partially answers the question left open in §VI.C (about the appearance of irreversibility in the diffusion limit).

Continuous time Markov chain

We are given

(i) a finite set Σ (called the *state space*)

and

(ii) a function

$$p : [0, \infty) \times \Sigma \times \Sigma \to [0, 1]$$

such that

$$t \mapsto p(t, \xi, \eta) \text{ is } C^1 \qquad (\xi, \eta \in \Sigma), \tag{1}$$

$$p(0, \xi, \eta) = \delta_\xi(\eta) = \begin{cases} 1 & \eta = \xi \\ 0 & \text{otherwise,} \end{cases} \tag{2}$$

$$\sum_{\eta \in \Sigma} p(t, \xi, \eta) = 1, \tag{3}$$

and

$$p(t + s, \xi, \eta) = \sum_{\gamma \in \Sigma} p(t, \xi, \gamma) p(s, \gamma, \eta). \tag{4}$$

We call p a *Markov transition function* and (4) the *Chapman–Kolmogorov formula*.

1. Generators and semigroups

Definitions. (i) Define

$$c : \Sigma \times \Sigma \to \mathbb{R}$$

by

$$c(\xi,\eta)=\lim_{t\to 0}\frac{p(t,\xi,\eta)-p(0,\xi,\eta)}{t}. \tag{5}$$

(ii) We further write

$$d(\xi,\eta)=\begin{cases} c(\xi,\eta) & \text{if } \xi\neq\eta \\ 0 & \text{if } \xi=\eta. \end{cases} \tag{6}$$

Remark. Owing to (2), (3),

$$c(\xi,\eta)\geq 0 \text{ if } \xi\neq\eta,\ \sum_{\eta} c(\xi,\eta)=0.$$

Thus

$$d(\xi,\eta)\geq 0.$$

□

Definitions. (i) If $f:\Sigma\to\mathbb{R}$, we define

$$Lf:\Sigma\to\mathbb{R}$$

by $[Lf](\xi)=\sum_\eta c(\xi,\eta)f(\eta)$, or equivalently

$$[Lf](\xi)=\sum_{\eta} d(\xi,\eta)(f(\eta)-f(\xi)) \qquad (\xi\in\Sigma). \tag{7}$$

We call L the *generator* of the Markov process.

(ii) We define also the *semigroup* $\{S(t)\}_{t\geq 0}$ generated by L by

$$[S(t)f](\xi)=\sum_{\eta} p(t,\xi,\eta)f(\eta). \tag{8}$$

Probabilistic interpretation. Think of a randomly jumping particle whose position at time $t\geq 0$ is $X(t)\in\Sigma$. Thus $\{X(t)\}_{t\geq 0}$ is a stochastic process and we may interpret $p(t,\xi,\eta)$ as the probability that $X(t)=\eta$, given that $X(0)=\xi$. According to (2), (5)

$$p(t,\xi,\eta)=\delta_\xi(\eta)+tc(\xi,\eta)+o(t) \text{ as } t\to 0;$$

and so if $\xi\neq\eta$, $c(\xi,\eta)$ *is the rate of jumps/unit time from* ξ *to* η. Furthermore

$$[S(t)f](\xi)=E(f(X(t))\mid X(0)=\xi)),$$

the expected value of $f(X(t))$, given that $X(0) = \xi$. Owing to (4) $\{X(t)\}_{t\geq 0}$ is a continuous time Markov process, with generator L. □

Properties of $S(t)$. For $s, t \geq 0$, we have

$$\left\{ \begin{array}{rcl} S(0) & = & I,\ S(t+s) = S(t)S(s) = S(s)S(t), \\ \frac{d}{dt}(S(t)f) & = & L(S(t)f) = S(t)(Lf),\ S(t)\mathbb{1} = \mathbb{1}, \end{array} \right. \tag{9}$$

where $\mathbb{1}$ denotes the function identically equal to 1 on Σ.

Definition. Let μ be a probability measure on Σ. We define then the probability measure $S^*(t)\mu$ by requiring

$$\int_\Sigma S(t)f d\mu = \int_\Sigma f dS^*(t)\mu \qquad (t \geq 0) \tag{10}$$

for each $f : \Sigma \to \mathbb{R}$. We call $\{S^*(t)\}_{t\geq 0}$ the *dual semigroup*.

Now fix a reference probability measure π on Σ, with

$$\pi(\eta) > 0 \text{ for all } \eta \in \Sigma.$$

Notation. Given a probability measure μ, write

$$\rho(\cdot, t) = \frac{dS^*(t)\mu}{d\pi}; \tag{11}$$

so that

$$[S^*(t)\mu](\eta) = \rho(\eta, t)\pi(\eta) \qquad (\eta \in \Sigma,\ t \geq 0). \tag{12}$$

Lemma. *We have*

$$\frac{\partial \rho}{\partial t} = L^*\rho \qquad \text{on } \ \Sigma \times [0, \infty), \tag{13}$$

where L^* is the adjoint of L with respect to π.

We call (13) the *forward equation*.

Proof. Let us first note

$$\begin{array}{rcl} \int_\Sigma \rho f d\pi & = & \int_\Sigma f dS^*(t)\mu \\ & = & \int_\Sigma S(t)f d\mu. \end{array}$$

Thus

$$\begin{aligned}\int_\Sigma \frac{\partial \rho}{\partial t} f d\pi &= \frac{d}{dt}\left(\int_\Sigma S(t) f d\mu\right) \\ &= \int_\Sigma S(t) L f d\mu \\ &= \int_\Sigma L f dS^*(t)\mu \\ &= \int_\Sigma L f \rho(\cdot, t) d\pi \\ &= \int_\Sigma f L^* \rho d\pi.\end{aligned}$$

This identity is valid for all $f : \Sigma \to \mathbb{R}$ and so (13) follows. □

2. Entropy production

Definition. We say the probability measure π is *invariant* provided

$$S^*(t)\pi = \pi \qquad \text{for all } t \geq 0. \tag{14}$$

Remark. It is easy to see that π is invariant if and only if

$$\int_\Sigma L f d\pi = 0 \tag{15}$$

or, equivalently,

$$\int_\Sigma S(t) f d\pi = \int_\Sigma f d\pi \tag{16}$$

for all $f : \Sigma \to \mathbb{R}$. □

We wish to identify circumstances under $S^*(t)\mu$ converges to an invariant measure as $t \to \infty$. The key will be certain estimates about the rate of entropy production.

Definition. Let π be a probability measure on Σ, with $\pi(\eta) > 0$ for each $\eta \in \Sigma$. If μ is another probability measure, we define the *entropy of μ with respect to π* to be

$$H(\mu, \pi) = \int_\Sigma \rho \log \rho d\pi, \tag{17}$$

where

$$\rho = d\mu / d\pi.$$

Remark. Since Σ is finite, (17) says

$$H(\mu, \pi) = \sum_\eta \log\left(\frac{\mu(\eta)}{\pi(\eta)}\right) \mu(\eta). \tag{18}$$

Clearly $\mu \mapsto H(\mu, \pi)$ is continuous. □

Lemma. *Let π be an invariant probability measure, with $\pi(\eta) > 0$ for all $\eta \in \Sigma$. Take μ to be any probability measure. Then*

$$\frac{d}{dt} H(S^*(t)\mu, \pi) \leq 0. \tag{19}$$

Proof. 1. Write

$$\phi(x) := x \log x - x + 1 \qquad (x \geq 0).$$

As noted in §VII,

$$\phi \text{ is convex, } \phi \geq 0 \text{ for } x \geq 0. \tag{20}$$

2. Take any π and set $\rho(\cdot, t) = dS^*(t)\mu/d\pi$. Assume $\rho(\cdot, t) > 0$. Then

$$\begin{aligned} \tfrac{d}{dt} H(S^*(t)\mu, \pi) &= \tfrac{d}{dt} \left(\textstyle\int_\Sigma \rho \log \rho d\pi \right) \\ &= \textstyle\int_\Sigma \frac{\partial \rho}{\partial t} \log \rho d\pi + \int_\Sigma \rho_t d\pi \\ &= \textstyle\int_\Sigma (L^* \rho) \log \rho d\pi + \int_\Sigma L^* \rho d\pi. \end{aligned}$$

Now

$$\int_\Sigma L^* \rho d\pi = \int_\Sigma g(L\mathbb{1}) d\pi = 0,$$

owing to (7). Thus

$$\begin{aligned} \tfrac{d}{dt} H(S^*(t)\mu, \pi) &= \textstyle\int_\Sigma \rho L(\log \rho) d\pi \\ &= \textstyle\sum_\xi \rho(\xi, t) \left(\sum_\eta d(\xi, \eta) \log \left(\frac{\rho(\eta, t)}{\rho(\xi, t)} \right) \right) \pi(\xi) \\ &= -\textstyle\sum_{\xi, \eta} d(\xi, \eta) \frac{\rho(\xi, t)}{\rho(\eta, t)} \log \left(\frac{\rho(\xi, t)}{\rho(\eta, t)} \right) \pi(\xi) \rho(\eta, t) \\ &= -\textstyle\sum_{\xi, \eta} d(\xi, \eta) \phi \left(\frac{\rho(\xi, t)}{\rho(\eta, t)} \right) \pi(\xi) \rho(\eta, t) \\ &+ \textstyle\sum_{\xi, \eta} d(\xi, \eta)(\rho(\xi, t) - \rho(\eta, t)\pi(\xi)). \end{aligned}$$

The last expression is

$$-\int_\Sigma L\rho(\cdot, t) d\pi = 0,$$

since π is invariant. Since $\phi \geq 0$, estimate (19) results.

If ρ is not everywhere positive, we omit the sites where $\rho = 0$ in the foregoing calculation. □

Remark. We call

$$G(t) = \sum_{\xi,\eta} d(\xi,\eta)\phi\left(\frac{\rho(\xi,t)}{\rho(\eta,t)}\right)\pi(\xi)\rho(\eta,t) \geq 0 \tag{21}$$

the *rate of entropy production at time t*. Then

$$\frac{d}{dt}H(S^*(t)\mu,\pi) = -G(t) \leq 0.$$

□

3. Convergence to equilibrium

Definition. The Markov chain is called *irreducible* if

$$p(t,\xi,\eta) > 0 \qquad (t>0,\ \xi,\eta) \in \Sigma. \tag{22}$$

Remark. It is straightforward to show that the Markov chain is irreducible if and only if for each pair $\xi,\eta \in \Sigma$, $\xi \neq \eta$ there exists a "path"

$$\xi = \gamma_0, \gamma_1, \ldots, \gamma_m = \eta$$

with

$$d(\gamma_i, \gamma_{i+1}) > 0 \qquad (i = 0, \ldots, m-1).$$

□

Theorem. *Assume the Markov chain is irreducible. Then*

(i) *there exists a unique invariant probability measure* $\pi > 0$,
and

(ii) *for each probability measure* μ,

$$\lim_{t\to\infty} S^*(t)\mu = \pi. \tag{23}$$

Proof. 1. First we build π. Fix any site $\xi_0 \in \Sigma$ and write

$$\pi(t,\eta) = \frac{1}{t}\int_0^t p(s,\xi_0,\eta)ds \qquad (t>0).$$

Define then

$$\pi(\eta) := \lim_{t_k\to\infty} \pi(t_k,\eta) \tag{24}$$

the sequence $t_k \to \infty$ selected so that the limit (24) exists for each $\eta \in \Sigma$. Clearly

$$0 \le \pi(\eta) \le 1, \ \sum_{\eta} \pi(\eta) = 1. \tag{25}$$

2. In addition, if $h > 0$ the Chapman–Kolmogorov formula (4) implies

$$\begin{aligned} \sum_\gamma \left(\tfrac{1}{t} \int_0^t p(s, \xi_0, \gamma) ds \right) p(h, \gamma, \eta) &= \tfrac{1}{t} \int_0^t p(s+h, \xi_0, \eta) ds \\ &= \tfrac{1}{t} \int_h^{t+h} p(s, \xi_0, \eta) ds \\ &= \tfrac{1}{t} \int_0^t p(s, \xi_0, \eta) ds + \tfrac{1}{t} \int_t^{t+h} p(s, \xi_0, \eta) ds - \tfrac{1}{t} \int_0^h p(s, \xi_0, \eta) ds. \end{aligned}$$

Let $t = t_k \to \infty$ and recall (24):

$$\sum_\gamma \pi(\gamma) p(h, \gamma, \eta) = \pi(\eta) \qquad (\eta \in \Sigma). \tag{26}$$

Then (25) and the irreducibility condition (22) imply

$$\pi(\eta) > 0 \text{ for each } \eta \in \Sigma. \tag{27}$$

Next differentiate (26) with respect to h and set $h = 0$:

$$\sum_\gamma \pi(\gamma) c(\gamma, \eta) = 0 \qquad (\eta \in \Sigma).$$

This identity implies

$$\int_\Sigma L f d\pi = \sum_{\xi, \eta} c(\xi, \eta) f(\eta) \pi(\xi) = 0$$

for all $f : \Sigma \to \mathbb{R}$ and so

$$\pi \text{ is an invariant measure.}$$

3. Next fix any ξ and define

$$\delta_\xi(\eta) = \begin{cases} 1 & \text{if } \eta = \xi \\ 0 & \text{if } \eta \ne \xi. \end{cases}$$

Then

$$p(t, \xi, \cdot) = S^*(t) \delta_\xi. \tag{28}$$

According to the Lemma,

$$t \mapsto H(p(t, \xi, \cdot), \pi) \text{ is nonincreasing in } t. \tag{29}$$

Now select any sequence $t_l \to \infty$ such that the limit

$$\nu(\eta) := \lim_{t_l \to \infty} p(t_l, \xi, \eta) \tag{30}$$

exists for each $\eta \in \Sigma$. Then (29) implies

$$\begin{aligned} \inf_{t \geq 0} H(p(t, \xi, \cdot), \pi) &= \lim_{t \to \infty} H(p(t, \xi, \cdot), \pi) \\ &= \lim_{t_l \to \infty} H(p(t_l, \xi, \cdot), \pi) \\ &= H(\nu, \pi). \end{aligned}$$

Also

$$\begin{aligned} S^*(t)\nu &= \lim_{t_l \to \infty} S^*(t) S^*(t_l) \delta_\xi \\ &= \lim_{t_l \to \infty} S(t + t_l) \delta_\xi \\ &= \lim_{t_l \to \infty} p(t + t_l, \xi, \cdot). \end{aligned}$$

Consequently

$$\begin{aligned} H(S^*(t)\nu, \pi) &= \lim_{t_l \to \infty} H(p(t + t_l, \xi, \cdot), \pi) \\ &= H(\nu, \pi). \end{aligned}$$

Thus

$$t \mapsto H(S^*(t)\nu, \pi) \text{ is constant.} \tag{31}$$

Set

$$\rho(\cdot, t) = dS^*(t)\nu / d\pi > 0.$$

Then (21), (31) imply the rate of entropy production

$$G(t) = \sum_{\xi, \eta} d(\xi, \eta) \phi \left(\frac{\rho(\xi, t)}{\rho(\eta, t)} \right) \pi(\xi) \rho(\eta, t) = 0$$

for $t \geq 0$. Since $\pi, \rho > 0$, we have

$$\begin{cases} \phi \left(\frac{\rho(\xi, t)}{\rho(\eta, t)} \right) = 0 \text{ and so } \rho(\xi, t) = \rho(\eta, t) \\ \text{for each } \xi, \eta \text{ with } d(\xi, \eta) > 0. \end{cases}$$

The Remark after (22) thus implies $\rho(\cdot, t)$ is constant and so

$$S^*(t)\nu = \pi \text{ for all } t \geq 0.$$

So $\nu = \pi$ and therefore

$$S^*(t)\delta_\xi \to \pi$$

for each $\xi \in \Sigma$. Assertion (23) follows. □

B. Large deviations

1. Thermodynamic limits

We turn next to the theory of *large deviations*, which will provide links between certain limit problems in probability, statistical mechanics, and various linear and nonlinear PDE.

Physical motivation. To motivate the central issues, let us first recall from Chapter VII these formulas for the canonical distribution:

$$F = -\frac{1}{\beta}\log Z,\ Z = \int_\Omega e^{-\beta H} d\pi.$$

Now it is most often the case in statistical mechanics that we are interested in a sequence of free energies and partition functions:

$$F_N = -\frac{1}{\beta}\log Z_N,\ Z_N = \int_{\Omega_N} e^{-\beta H_N} d\pi_N \qquad (N = 1, 2, \dots). \tag{1}$$

Typically (1) represents the free energy and partition function for a system of N interacting particles (described by microstates in the system $(\Omega_N, \mathcal{F}_N, \pi_N)$, with Hamiltonian $H_N : \Omega_N \to \mathbb{R}$). We often wish to compute the limit as $N \to \infty$ of the *free energy per particle*:

$$f(\beta) = \lim_{N\to\infty} \frac{1}{N} F_N = -\lim_{N\to\infty} \frac{1}{\beta N}\log Z_N. \tag{2}$$

Understanding in various models the behavior of the mapping $\beta \mapsto f(\beta)$ is a central problem in statistical mechanics; see for instance Thompson [T, §3.6]. We call (2) a *thermodynamic limit*.

To help us understand the mathematical and physical issues here, let us rewrite

$$Z_N = \int_{\Omega_N} e^{-\beta H_N} d\pi_N = \int_\Sigma e^{-N\beta\xi} dP_N,$$

where the state space Σ is $\mathbb{R}^1$ and P_N is the distribution of $\frac{1}{N}H_N$ on Σ; that is,

$$P_N(-\infty, \gamma] = \pi_N\left(\omega \in \Omega_N \mid \frac{H_N(\omega)}{N} \le \gamma\right) \tag{3}$$

for $\gamma \in \mathbb{R}^1$. Setting

$$\varepsilon = \frac{1}{N},$$

we recast (2) as

$$f(\beta) = -\frac{1}{\beta} \lim_{\varepsilon \to 0} \varepsilon \log \left(\int_\Sigma e^{-\frac{\beta \xi}{\varepsilon}} dP_\varepsilon \right). \tag{4}$$

Let us next suppose that for small $\varepsilon > 0$:

$$dP_\varepsilon \approx e^{-I/\varepsilon} dQ \tag{5}$$

in some unspecified sense, where $I : \Sigma \to \mathbb{R}$, Q is a reference measure on Σ. Inserting (5) into (4), we may expect that

$$\lim_{\varepsilon \to 0} \varepsilon \log \left(\int_\Sigma e^{\frac{-\beta \xi - I(\xi)}{\varepsilon}} dQ \right) = \sup_\xi (-\beta \xi - I(\xi)).$$

Consequently—supposing the foregoing computations are somehow legitimate—we deduce

$$f(\beta) = \frac{1}{\beta} \inf_\xi (\beta \xi + I(\xi)) \quad (\beta \in \mathbb{R}). \tag{6}$$

What is the physical meaning of this formula? First note that the *energy per particle* is

$$\begin{aligned} \tfrac{1}{N} E_N &= \tfrac{1}{N} \langle H_N \rangle \\ &= \tfrac{1}{N} \textstyle\int_{\Omega_N} H_N e^{-\beta H_N} \frac{d\mu_N}{Z_N} \\ &= \textstyle\int_\Sigma \xi e^{-N\beta\xi} \frac{dP_N}{Z_N} \\ &= \textstyle\int_\Sigma \xi e^{-\frac{\beta\xi}{\varepsilon}} \frac{dP_\varepsilon}{Z_\varepsilon} \\ &\approx \textstyle\int_\Sigma \xi e^{\frac{-\beta\xi - I(\xi)}{\varepsilon}} \frac{dQ}{Z_\varepsilon}. \end{aligned}$$

Hence as $N \to \infty$, we may expect

$$\frac{E_N}{N} \to e, \tag{7}$$

where

$$\beta e + I(e) = \inf_\xi (\beta \xi + I(\xi)). \tag{8}$$

Let us therefore interpret e as the *energy* in the thermodynamic limit.

Next recall from §VIII.C.3 the formula

$$\log Z = \sup_E \left(-\beta E + \frac{S}{k} \right),$$

and remember

$$F = -\frac{1}{\beta} \log Z.$$

Thus

$$-\beta F = \sup_E \left(-\beta E + \frac{S}{k} \right). \tag{9}$$

On the other hand, (6) says

$$-\beta f = \sup_\xi (-\beta \xi - I(\xi)). \tag{10}$$

In view of (8)–(10) we might then conjecture that

$$\left(-\frac{S}{k} \right)^{**} = I^{**},$$

S denoting the entropy and * the Legendre transform. As S is presumably concave, we deduce then

$$S = -kI^{**}. \tag{11}$$

Should I also be convex, then (11) reduces to

$$S = -kI. \tag{12}$$

In this case our supposition (5), which we now rewrite as

$$dP_\varepsilon \approx e^{\frac{S}{k\varepsilon}} dQ, \tag{13}$$

says that *entropy S controls the asymptotics of $\{P_\varepsilon\}_{0<\varepsilon\leq 1}$ in the thermodynamic limit* and that *the most likely states for small $\varepsilon > 0$ are those which maximize the entropy.*

2. Basic theory

We now follow Donsker–Varadhan (see e.g. Varadhan [V], Dembo–Zeitouni [D-Z], etc.) and provide a general probabilistic framework within which to understand and generalize the foregoing heuristics.

a. Rate functions

Notation. Hereafter

Σ denotes a separable, complete, metric space,

and

$$\{P_\varepsilon\}_{0<\varepsilon\leq 1} \text{ is a family of Borel probability measures on } \Sigma.$$

□

Definition. We say that $\{P_\varepsilon\}_{0<\varepsilon\leq 1}$ satisfies the *large deviation principle* with *rate function* I provided

(i) $I : \Sigma \to [0, \infty]$ is lower semicontinuous, $I \not\equiv +\infty$,

(ii) for each $l \in \mathbb{R}$,

$$\text{the set } \{\xi \in \Sigma \mid 0 \leq I(\xi) \leq l\} \text{ is compact,} \tag{14}$$

(iii) for each closed set $C \subseteq \Sigma$,

$$\limsup_{\varepsilon\to 0} \varepsilon \log P_\varepsilon(C) \leq -\inf_C I \tag{15}$$

and

(iv) for each open set $U \subseteq \Sigma$,

$$\liminf_{\varepsilon\to 0} \varepsilon \log P_\varepsilon(U) \geq -\inf_U I. \tag{16}$$

Remarks. (i) If E is a Borel subset of Σ for which

$$\inf_{E^0} I = \inf_E I = \inf_{\bar{E}} I,$$

then

$$\lim_{\varepsilon\to 0} \varepsilon \log P_\varepsilon(E) = -\inf_E I.$$

This gives a precise meaning to the heuristic (5) from the previous section (without the unnecessary introduction of the reference measure).

(ii) The rate function I is called the *entropy function* in Ellis [EL]. This book contains clear explanations of the connections with statistical mechanics.

(iii) It is sometimes convenient to consider instead of $\varepsilon \to 0$ an index $n \to \infty$. Thus we say $\{P_n\}_{n=1}^\infty$ satisfies the large deviation principle with rate function I if

$$\begin{cases} \limsup_{n\to\infty} \frac{1}{n} \log P_n(C) \leq -\inf_C I \quad (C \text{ closed}) \\ \text{and} \\ \liminf_{n\to\infty} \frac{1}{n} \log P_n(U) \geq -\inf_U I \quad (U \text{ open}). \end{cases} \tag{17}$$

□

b. Asymptotic evaluations of integrals

We now make clearer the connections between large deviation theory and the heuristics in §1.

Theorem 1. *Let* $\{P_\varepsilon\}_{0<\varepsilon\leq 1}$ *satisfy the large deviation principle with rate function* I. *Let*

$$g : \Sigma \to \mathbb{R}$$

be bounded, continuous. Then

$$\lim_{\varepsilon\to 0} \varepsilon \log \left(\int_\Sigma e^{\frac{g}{\varepsilon}} dP_\varepsilon \right) = \sup_\Sigma (g - I). \tag{18}$$

Proof. 1. Fix $\delta > 0$. We write

$$\Sigma = \bigcup_{i=1}^N C_i,$$

where each C_i is closed and the oscillation of g on C_i is less than or equal to δ $(i = 1, \ldots, N)$. (Assuming without loss that $g \geq 0$, we can for instance take

$$C_i = \{\xi \in \Sigma \mid (i-1)\delta \leq g(\xi) \leq i\delta\}.)$$

Then

$$\begin{array}{rcl} \int_\Sigma e^{\frac{g}{\varepsilon}} dP_\varepsilon & \leq & \sum_{i=1}^N \int_{C_i} e^{\frac{g}{\varepsilon}} dP_\varepsilon \\ & \leq & \sum_{i=1}^N \int_{C_i} e^{\frac{g_i+\delta}{\varepsilon}} dP_\varepsilon, \end{array}$$

where

$$g_i = \inf_{C_i} g \qquad (i = 1, \ldots, N).$$

Thus

$$\begin{array}{rcl} \log \left(\int_\Sigma e^{\frac{g}{\varepsilon}} dP_\varepsilon \right) & \leq & \log \left(N \max_{1\leq i\leq N} e^{\frac{g_i+\delta}{\varepsilon}} P_\varepsilon(C_i) \right) \\ & = & \log N + \max_{1\leq i\leq N} \left[\left(\frac{g_i+\delta}{\varepsilon} \right) + \log P_\varepsilon(C_i) \right], \end{array}$$

and so (15) implies

$$\begin{array}{rcl} \limsup_{\varepsilon\to 0} \varepsilon \log \left(\int_\Sigma e^{\frac{g}{\varepsilon}} dP_\varepsilon \right) & \leq & \max_{1\leq i\leq N} \left[(g_i + \delta) - \inf_{C_i} I \right] \\ & \leq & \max_{1\leq i\leq N} \sup_{C_i} (g - I) + \delta \\ & = & \sup_\Sigma (g - I) + \delta. \end{array}$$

Consequently

$$\limsup_{\varepsilon\to 0} \varepsilon \log \left(\int_\Sigma e^{\frac{g}{\varepsilon}} dP_\varepsilon \right) \leq \sup_\Sigma (g - I). \tag{19}$$

2. Again fix $\delta > 0$. There exists $\eta \in \Sigma$ with

$$g(\eta) - I(\eta) \geq \sup_{\Sigma}(g - I) - \frac{\delta}{2}. \tag{20}$$

Since g is continuous, there exists an open neighborhood U of η such that

$$g(\xi) \geq g(\eta) - \frac{\delta}{2} \text{ for } \xi \in U. \tag{21}$$

Then

$$\begin{aligned}
\liminf_{\varepsilon\to 0} \varepsilon \log\left(\int_\Sigma e^{\frac{g}{\varepsilon}} dP_\varepsilon\right) &\geq \liminf_{\varepsilon\to 0} \varepsilon \log\left(\int_U e^{\frac{g}{\varepsilon}} dP_\varepsilon\right) \\
&\geq \liminf_{\varepsilon\to 0} \varepsilon \log\left(\int_U e^{\frac{g(\eta)-\frac{\delta}{2}}{\varepsilon}} dP_\varepsilon\right) \text{ by (21)} \\
&= g(\eta) - \tfrac{\delta}{2} + \liminf_{\varepsilon\to 0} \varepsilon P_\varepsilon(U) \\
&\geq g(\eta) - \tfrac{\delta}{2} - \inf_U I \text{ by (16)} \\
&\geq g(\eta) - I(\eta) - \tfrac{\delta}{2} \\
&\geq \sup_\Sigma(g - I) - \delta \text{ by (20)}.
\end{aligned}$$

Hence

$$\liminf_{\varepsilon\to 0} \varepsilon \log\left(\int_\Sigma e^{\frac{g}{\varepsilon}} dP_\varepsilon\right) \geq \sup_{\Sigma}(g - I).$$

This bound and (19) finish the proof of (18). □

We will require in the next section the converse statement.

Theorem 2. *Assume the limit* (18) *holds for each bounded, Lipschitz function* $g : \Sigma \to \mathbb{R}$, *where* $I : \Sigma \to [0, \infty]$ *is lower semicontinuous,* $I \not\equiv +\infty$. *Suppose also the sets* $\{0 \leq I \leq l\}$ *are compact for each* $l \in \mathbb{R}$.

Then $\{P_\varepsilon\}_{0<\varepsilon\leq 1}$ *satisfies the large deviation principle with rate function* I.

Proof. We must prove (15), (16)

1. Let $C \subseteq \Sigma$ be closed and set

$$g_m(\xi) = \max(-m, -m \text{ dist}(\xi, C)) \qquad (m = 1, \dots). \tag{22}$$

Then g_m is bounded, Lipschitz and

$$\varepsilon \log\left(\int_\Sigma e^{g_m/\varepsilon} dP_\varepsilon\right) \geq \varepsilon \log P^\varepsilon(C).$$

Thus

$$\begin{aligned}
\limsup_{\varepsilon\to 0} \varepsilon \log P^\varepsilon(C) &\leq \lim_{\varepsilon\to 0} \varepsilon \log\left(\int_\Sigma e^{g_m/\varepsilon} dP_\varepsilon\right) \\
&= \sup_\Sigma(g_m - I).
\end{aligned}$$

Let $m \to \infty$, noting from (21) that

$$\sup_{\Sigma}(g_m - I) \to \sup_{C}(-I) = -\inf_{C} I,$$

since C is closed and I is lower semicontinuous. The limit (15) is proved.

2. Next suppose $U \subseteq \Sigma$ open and take

$$C_k = \left\{ \xi \in U \mid \ \operatorname{dist}(\xi, \Sigma - U) \geq \frac{1}{k} \right\}.$$

Then $C_k \subset U$, C_K is closed ($k = 1, \dots$). Define

$$g_m(\xi) = k \max\left(-\frac{m}{k}, -m \operatorname{dist}(\xi, C_k) \right).$$

Note that

$$-m \leq g_m \leq 0, \ g_m = 0 \text{ on } C_k, \ g_m = -m \text{ on } \Sigma - U.$$

Then

$$\begin{aligned} \varepsilon \log\left(\textstyle\int_\Sigma e^{g_m/\varepsilon} dP_\varepsilon \right) &\leq \varepsilon \log(P_\varepsilon(U) + e^{-m/\varepsilon} P_\varepsilon(\Sigma - U)) \\ &\leq \varepsilon \log(P_\varepsilon(U) + e^{-m/\varepsilon}). \end{aligned}$$

Thus

$$\begin{aligned} \sup_{C_k}(-I) &\leq \sup_{\Sigma}(g_m - I) \\ &= \lim_{\varepsilon \to 0} \varepsilon \log\left(\textstyle\int_\Sigma e^{g_m/\varepsilon} dP_\varepsilon \right) \\ &\leq \liminf_{\varepsilon \to 0} \varepsilon \log(P_\varepsilon(U) + e^{-m/\varepsilon}). \end{aligned} \tag{23}$$

But

$$\begin{aligned} \varepsilon \log(P_\varepsilon(U) + e^{-m/\varepsilon}) &\leq \varepsilon \log(2 \max(P_\varepsilon(U), e^{-m/\varepsilon}) \\ &= \varepsilon \log 2 + \max(\varepsilon \log P_\varepsilon(U), -m), \end{aligned}$$

and so

$$\liminf_{\varepsilon \to 0} \varepsilon \log(P_\varepsilon(U) + e^{-m/\varepsilon}) \leq \max\left(\liminf_{\varepsilon \to 0} \varepsilon \log P_\varepsilon(U), -m \right).$$

Combining this calculation with (23) and sending $m \to \infty$, we deduce

$$-\inf_{C_k} I \leq \liminf_{\varepsilon \to 0} \varepsilon \log P_\varepsilon(U).$$

Since $U = \bigcup_{k=1}^{\infty} C_k$, the limit (16) follows. □

C. Cramer's Theorem

In this section we illustrate the use of PDE methods by presenting an unusual proof, due to R. Jensen, of Cramer's Theorem, characterizing large deviations for sums of i.i.d. random variables.

More precisely, take $(\Omega, \mathcal{F}, \pi)$ to be a probability space and suppose

$$\text{(1)} \qquad \begin{cases} \mathbf{Y}_k : \Omega \to \mathbb{R}^m \qquad (k = 1, \dots) \\ \text{are independent, identically distributed} \\ \text{random variables.} \end{cases}$$

We write $\mathbf{Y} = \mathbf{Y}_1$ and assume as well that

$$\text{(2)} \qquad \begin{cases} \text{the exponential generating function } Z = E(e^{p \cdot \mathbf{Y}}) \\ \text{is finite for each } p \in \mathbb{R}^m, \end{cases}$$

where $E(\cdot)$ denotes expected value. Thus

$$Z = \int_\Omega e^{p \cdot \mathbf{Y}} d\pi.$$

We turn attention now to the partial sums

$$\text{(3)} \qquad \mathbf{S}_n = \frac{\mathbf{Y}_1 + \cdots + \mathbf{Y}_n}{n}$$

and their distributions P_n on $\Sigma = \mathbb{R}^m$ $(n = 1, \dots)$.

Next define

$$\text{(4)} \qquad F := \log Z,$$

that is,

$$\text{(5)} \qquad F(p) = \log E(e^{p \cdot \mathbf{Y}}) = \log \left(\int_\Omega e^{p \cdot \mathbf{Y}} d\pi \right).$$

We introduce also the Legendre transform of F:

$$\text{(6)} \qquad L(q) = \sup_{p \in \mathbb{R}^m} (p \cdot q - F(p)) \qquad (q \in \mathbb{R}^m)$$

which turns out to be the rate function:

Theorem. *The probability measures* $\{P_n\}_{n=1}^\infty$ *satisfy the large deviation principle with rate function* $I(\cdot) = L(\cdot)$.

Remark. By the Law of Large Numbers

$$\mathbf{S}_n \to E(\mathbf{Y}) =: y \text{ a.s. as } n \to \infty.$$

As we will compute in the following proof,

$$DF(0) = y$$

and so

$$DL(y) = 0,$$

provided L is smooth at y. Hence $x \mapsto L$ has its minimum at y, and in fact

$$\begin{cases} L(y) = 0 \\ L(x) > 0 \quad (x \neq y) \end{cases}$$

Take a Borel set E. Assuming

$$\inf_{E^0} L = \inf_{E} L = \inf_{\bar{E}} L,$$

we deduce

$$P_n(E) = e^{n(-\inf_E L + o(1))}.$$

So if $y \notin \bar{E}$, $P_n(E) \to 0$ exponentially fast as $n \to \infty$. □

Proof. 1. Write $\mathbf{Y} = (Y^1, \dots, Y^m)$. Then for $1 \leq k, l \leq m$:

$$\begin{array}{rcl} \frac{\partial F}{\partial p_k} & = & \frac{E(Y^k e^{p\cdot \mathbf{Y}})}{E(e^{p\cdot \mathbf{Y}})}, \\ \frac{\partial^2 F}{\partial p_k \partial p_l} & = & \frac{E(Y^k Y^l e^{p\cdot \mathbf{Y}})}{E(e^{p\cdot \mathbf{Y}})} - \frac{E(Y^k e^{p\cdot \mathbf{Y}}) E(Y^l e^{p\cdot \mathbf{Y}})}{E(e^{p\cdot \mathbf{Y}})^2}. \end{array}$$

Thus if $\xi \in \mathbb{R}^m$,

$$\begin{array}{rcl} \sum_{k,l=1}^m F_{p_k p_l} \xi_k \xi_l & = & \frac{E((\mathbf{Y}\cdot\xi)^2 e^{p\cdot \mathbf{Y}}) E(e^{p\cdot \mathbf{Y}}) - E((\mathbf{Y}\cdot\xi) e^{p\cdot \mathbf{Y}})^2}{E(e^{p\cdot \mathbf{Y}})^2} \\ & \geq & 0, \end{array}$$

since

$$E((\mathbf{Y}\cdot\xi) e^{p\cdot \mathbf{Y}}) \leq E((\mathbf{Y}\cdot\xi)^2 e^{p\cdot \mathbf{Y}})^{1/2} E(e^{p\cdot \mathbf{Y}})^{1/2}.$$

Hence

$$p \mapsto F(p) \text{ is smooth, convex.} \tag{7}$$

Clearly also

$$F(0) = \log E(e^0) = 0. \tag{8}$$

Define L by the Legendre transformation (6). Then

$$L(q) = \sup_p (p \cdot q - F(p)) \geq -F(0) = 0$$

for all q, and so

$$\text{(9)} \qquad \begin{cases} L : \mathbb{R}^m \to [0, \infty] \text{ is convex, lower} \\ \text{semicontinuous.} \end{cases}$$

In addition

$$\lim_{|q| \to \infty} \frac{L(q)}{|q|} = \infty$$

(cf. [E1, §III.3]), and thus for each $l \in \mathbb{R}$,

$$\text{(10)} \qquad \text{the set } \{q \in \mathbb{R}^m \mid 0 \leq L(q) \leq l\} \text{ is compact.}$$

2. Next take $g : \mathbb{R}^m \to \mathbb{R}$ to be bounded, Lipschitz. We intend to prove

$$\text{(11)} \qquad \lim_{n \to \infty} \frac{1}{n} \log \left(\int_{\mathbb{R}^m} e^{ng} dP_n \right) = \sup_{\mathbb{R}^m} (g - L),$$

where P_n is the distribution of $\mathbf{S}_n = \frac{\mathbf{Y}_1 + \cdots + \mathbf{Y}_n}{n}$ on $\mathbb{R}^m$. The idea is to associate somehow the left hand side of (11) with the unique viscosity solution of the Hamilton–Jacobi PDE

$$\text{(12)} \qquad \begin{cases} u_t - F(Du) = 0 \quad \text{in } \mathbb{R}^m \times (0, \infty) \\ \qquad\qquad u = g \quad \text{on } \mathbb{R}^m \times \{t = 0\}. \end{cases}$$

The right hand side of (11) will appear when we invoke the Hopf–Lax formula for the solution of (12).

To carry out this program, we fix any point $x \in \mathbb{R}^m$ and then write

$$t_k = k/n \qquad (k = 0, \dots).$$

We define

$$\text{(13)} \qquad w_n(x, t_k) := E \left(h_n \left(\frac{\mathbf{Y}_1 + \cdots + \mathbf{Y}_k}{n} + x \right) \right),$$

where

$$\text{(14)} \qquad h_n := e^{ng}.$$

3. We first *claim*:

$$\text{(15)} \qquad w_n(x, t_{k+1}) = E \left(w_n \left(x + \frac{\mathbf{Y}_{k+1}}{n}, t_k \right) \right) \qquad (k = 0, \dots).$$

This identity is valid since the random variables $\{\mathbf{Y}_k\}_{k=1}^{\infty}$ are independent. Indeed,

$$\begin{aligned} w_n(x,t_{k+1}) &= E\left(h_n\left(\tfrac{\mathbf{Y}_1+\cdots+\mathbf{Y}_k}{n}+\tfrac{\mathbf{Y}_{k+1}}{n}+x\right)\right) \\ &= E\left(E\left(h_n\left(\tfrac{\mathbf{Y}_1+\cdots+\mathbf{Y}_k}{n}+\tfrac{\mathbf{Y}_{k+1}}{n}+x\right)\Big|\,\mathbf{Y}_{k+1}\right)\right) \\ &= E\left(w_n\left(\tfrac{\mathbf{Y}_{k+1}}{n}+x,t_k\right)\right), \end{aligned}$$

the last equality holding by independence. More precisely, we used here the formula

$$E(\phi(X,Y)\mid Y)=\psi(Y) \text{ a.s.},$$

where X, Y are independent random variables, ϕ is continuous, bounded, and

$$\psi(y):=E(\phi(X,y)).$$

See, e.g., Breiman [BN, §4.2].

4. Next define

$$u_n(x,t_k):=\frac{1}{n}\log w_n(x,t_k) \tag{16}$$

for $n=1,\ldots, k=0,\ldots$. We assert next that

$$\|u_n\|_{L^\infty}\le\|g\|_{L^\infty},\ \|Du_n\|_{L^\infty}\le\|Dg\|_{L^\infty}, \tag{17}$$

D as usual denoting the gradient in the spatial variable x. Let us check (17) by first noting from (13), (14) that

$$\|w_n\|_{L^\infty}\le\|h_n\|_{L^\infty}=e^{n\|g\|_{L^\infty}}.$$

The first inequality in (17) follows. Now fix a time $t_k=\frac{k}{n}$. Then for a.e. $x\in\mathbb{R}^m$ we may compute from (13), (14) that

$$\begin{aligned} Dw_n(x,t_k) &= E\left(Dh_n\left(\tfrac{\mathbf{Y}_1+\cdots+\mathbf{Y}_k}{n}+x\right)\right) \\ &= nE\left(Dgh_n\left(\tfrac{X_1+\cdots+Y_k}{n}+x\right)\right). \end{aligned}$$

Consequently

$$\begin{aligned} |Dw_n| &\le n\|Dg\|_{L^\infty}E\left(h_n\left(\tfrac{\mathbf{Y}_1+\cdots+\mathbf{Y}_k}{n}+x\right)\right) \\ &= n\|Dg\|_{L^\infty}w_n. \end{aligned} \tag{18}$$

Recalling (16) we deduce the second inequality in (17).

Next take a point $x \in \mathbb{R}^m$ and compute:

$$\begin{aligned} w_n(x, t_{k+1}) &= E\left(e^{ng\left(\frac{\mathbf{Y}_1+\cdots+\mathbf{Y}_{k+1}}{n}+x\right)}\right) \\ &\leq E\left(e^{ng\left(\frac{\mathbf{Y}_1+\cdots+\mathbf{Y}_k}{n}+x\right)+\|Dg\|_{L^\infty}|\mathbf{Y}_{k+1}|}\right) \\ &= E\left(e^{ng\left(\frac{\mathbf{Y}_1+\cdots+\mathbf{Y}_k}{n}+x\right)}\right) E\left(e^{\|Dg\|_{L^\infty}|\mathbf{Y}_{k+1}|}\right) \end{aligned}$$

by independence. Thus

$$w_n(x, t_{k+1}) \leq w_n(x, t_k) E\left(e^{\|Dg\|_{L^\infty}|\mathbf{Y}|}\right) \tag{19}$$

for $\mathbf{Y} = \mathbf{Y}_1$, as the $\{\mathbf{Y}_k\}_{k=1}^\infty$ are identically distributed. Assumption (2) implies

$$E\left(e^{\|Dg\|_{L^\infty}|\mathbf{Y}|}\right) =: e^C < \infty.$$

Therefore (16), (19) imply:

$$u_n(x, t_{k+1}) - u_n(x, t_k) \leq \frac{1}{n} C,$$

and a similar calculation verifies that

$$u_n(x, t_{k+1}) - u_n(x, t_k) \geq -\frac{1}{n} C.$$

Consequently

$$|u_n(x, t_k) - u_n(x, t_l)| \leq C|t_k - t_l| \qquad (k, l \geq 1). \tag{20}$$

5. Extend $u_n(x, t)$ to be linear in t for $t \in [t_k, t_{k+1}]$ $(k = 0, \dots)$. Then estimates (17), (20) imply there exists a sequence $n_r \to \infty$ such that

$$u_{n_r} \to u \text{ locally uniformly in } \mathbb{R}^m \times [0, \infty). \tag{21}$$

Obviously $u = g$ on $\mathbb{R}^m \times \{t = 0\}$. We assert as well that *u is a viscosity solution of the* PDE

$$u_t - F(Du) = 0 \text{ in } \mathbb{R}^m \times (0, \infty). \tag{22}$$

To verify this, we recall the relevant definitions from Chapter VI, take any $v \in C^2(\mathbb{R}^m \times (0, \infty))$ and suppose

$$u - v \text{ has a strict local maximum at a point } (x_0, t_0).$$

We must prove:

$$v_t(x_0,t_0) - F(Dv(x_0,t_0)) \le 0. \tag{23}$$

We may also assume, upon redefining v outside some neighborhood of (x_0,t_0) if necessary, that $u(x_0,t_0) = v(x_0,t_0)$,

$$\sup |v, Dv, D^2 v| < \infty, \tag{24}$$

and $v > \sup(u^n)$ except in some region near (x_0,t_0). In view of (21) we can find for $n = n_r$ points (x_n, t_{k_n}), $t_{k_n} = \frac{k_n}{n}$, such that

$$u_n(x_n,t_{k_n}) - v(x_n,t_{k_n}) = \max_{x\in\mathbb{R}^m, k=0,\dots} [u_n(x,t_k) - v(x,t_k)] \tag{25}$$

and

$$(x_n,t_{k_n}) \to (x_0,t_0) \text{ as } n = n_r \to \infty. \tag{26}$$

Write

$$\alpha_n := u_n(x_n,t_{k_n}) - v(x_n,t_{k_n}). \tag{27}$$

Then for $n = n_r$:

$$\begin{aligned}
e^{n(\alpha_n + v(x_n,t_{k_n}))} &= e^{nu_n(x_n,t_{k_n})} \\
&= w_n(x_n,t_{k_n}) \text{ by (16)} \\
&= E\left(w_n\left(x_n + \tfrac{\mathbf{Y}_{k_n}}{n}, t_{k_n-1}\right)\right) \text{ by (15)} \\
&= E\left(e^{nu_n\left(x_n+\frac{\mathbf{Y}_{k_n}}{n}, t_{k_n-1}\right)}\right) \text{ by (16)} \\
&\le E\left(e^{n\left(\alpha_n + v\left(x_n+\frac{\mathbf{Y}_{k_n}}{n}, t_{k_n-1}\right)\right)}\right)
\end{aligned}$$

the last inequality holding according to (25), (27). Thus

$$e^{nv(x_n,t_{k_n})} \le E\left(e^{nv\left(x_n+\frac{\mathbf{Y}}{\mathbf{n}}, t_{k_n-1}\right)}\right)$$

for $n = n_r$. Now

$$v\left(x_n + \frac{\mathbf{Y}}{\mathbf{n}}, t_{k_n-1}\right) = v(x_n, t_{k_n-1}) + Dv(x_n,t_{k_n-1})\cdot\frac{\mathbf{Y}}{\mathbf{n}} + \beta_n,$$

where

$$\beta_n := v\left(x_n + \frac{\mathbf{Y}}{\mathbf{n}}, t_{k_n-1}\right) - v(x_n, t_{k_n-1}) - Dv(x_n, t_{k_n-1}) \cdot \frac{\mathbf{Y}}{\mathbf{n}}. \tag{28}$$

Thus

$$e^{nv(x_n,t_{k_n})} \leq e^{nv_n(x_n,t_{k_n-1})} E\left(e^{Dv(x_n,t_{k_n-1})\cdot\mathbf{Y}+n\beta_n}\right),$$

and hence

$$\frac{v(x_n, t_{k_n}) - v(x_n, t_{k_n-1})}{1/n} \leq \log E\left(e^{Dv(x_n,t_{k_n-1})\cdot\mathbf{Y}+n\beta_n}\right). \tag{29}$$

Now (24), (27) imply

$$\lim_{n\to\infty} n\beta_n = 0 \text{ a.s.},$$

and furthermore

$$\left|e^{Dv\cdot\mathbf{Y}+n\beta_n}\right| \leq e^{C|\mathbf{Y}|}.$$

Our assumption (2) implies also that $E(e^{C|\mathbf{Y}|}) < \infty$. We consequently may invoke the Dominated Convergence Theorem and pass to limits as $n = n_r \to \infty$:

$$\begin{aligned} v_t(x_0, t_0) &\leq \log E\left(e^{Dv(x_0,t_0)\cdot\mathbf{Y}}\right) \\ &= F(Dv(x_0, t_0)). \end{aligned}$$

This is (23), and the reverse inequality likewise holds should $u-v$ have a strict local minimum at a point (x_0, t_0). We have therefore proved u is a viscosity solution of (22). Since $u = g$ on $\mathbb{R}^m \times \{t = 0\}$, we conclude that u is the unique viscosity solution of the initial value problem (12). In particular $u^n \to u$.

6. We next transform (12) into a different form, by noting that $\tilde{u} = -u$ is the unique viscosity solution of

$$\begin{cases} \tilde{u}_t + \tilde{F}(D\tilde{u}) = 0 & \text{in } \mathbb{R}^m \times (0, \infty) \\ \tilde{u} = \tilde{g} & \text{on } \mathbb{R}^m \times \{t = 0\} \end{cases} \tag{30}$$

for

$$\tilde{g} = -g, \ \tilde{F}(p) = F(-p). \tag{31}$$

Indeed if $\tilde{u} - \tilde{v}$ has a local maximum at (x_0, t_0), then $u - v$ has a local minimum, where $v = -\tilde{v}$. Thus

$$v_t(x_0, t_0) - F(Dv(x_0, t_0)) \geq 0, \tag{32}$$

since u is a v is viscosity solution of (22). But $Dv = -D\tilde{v}$, $v_t = -\tilde{v}_t$. Consequently (32) says

$$\tilde{v}_t(x_0, t_0) + \tilde{F}(D\tilde{v}(x_0, t_0)) \le 0.$$

The reverse inequality obtains if $\tilde{u} - \tilde{v}$ has a local minimum at (x_0, t_0). This proves (30).

According to the Hopf–Lax formula from §V.B:

$$\tilde{u}(x,t) = \inf_y \left\{ t\tilde{L}\left(\frac{x-y}{t}\right) + \tilde{g}(y) \right\}, \tag{33}$$

where $\tilde{L}$ is the Legendre transform of the convex function $\tilde{F}$. But then

$$\begin{aligned} \tilde{L}(q) &= \sup_p (p \cdot q - \tilde{F}(p)) \\ &= \sup_p (p \cdot q - F(-p)) \\ &= \sup_p (p \cdot (-q) - F(p)) \\ &= L(-q). \end{aligned}$$

Therefore

$$\begin{aligned} u(x,t) &= -\tilde{u}(x,t) \\ &= \sup_y \left(-t\tilde{L}\left(\frac{x-y}{t}\right) - \tilde{g}(y) \right) \\ &= \sup_y \left\{ g(y) - tL\left(\frac{y-x}{t}\right) \right\}. \end{aligned}$$

In particular

$$u(0,1) = \sup_y \{g(y) - L(y)\}. \tag{34}$$

But

$$\begin{aligned} u_n(0,1) &= \tfrac{1}{n} \log w_n(0, t_n) \\ &= \tfrac{1}{n} \log E\left(h_n\left(\tfrac{\mathbf{Y}_1 + \cdots + \mathbf{Y}_n}{n} \right) \right) \\ &= \tfrac{1}{n} \log E\left(e^{ng(\mathbf{S}_n)} \right) \\ &= \tfrac{1}{n} \log \left(\textstyle\int_{\mathbb{R}^m} e^{ng} dP_n \right). \end{aligned} \tag{35}$$

As $u_n(0,1) \to u(0,1)$, (34) and (35) confirm the limit (11).

The second theorem in §B thus implies that $I = L$ is the rate function for $\{P_n\}_{n=1}^{\infty}$.

□

Remark. This proof illustrates the vague belief that rate functions, interpreted as functions of appropriate parameters, are viscosity solutions of Hamilton–Jacobi type nonlinear PDE.

The general validity of this principle is unclear, but there are certainly many instances in the research literature. See for instance the next section of these notes, and look also in the book by Freidlin–Wentzell [F-W].

If we accept from §B.1 the identification of rate functions and entropy (up to a minus sign and Boltzmann's constant), then the foregoing provides us with a quite new interplay between entropy ideas and nonlinear PDE. □

D. Small noise in dynamical systems

In this last section we discuss another PDE approach to a large deviations problem, this involving the small noise asymptotics of stochastic ODE.

1. Stochastic differential equations

We rapidly recount in this subsection the rudiments of stochastic ODE theory: see, e.g., Arnold [A], Freidlin [FR] or Oksendal [OK] for more.

Notation. (i) $(\Omega, \mathcal{F}, \pi)$ is a probability space.

(ii) $\{\mathbf{W}(t)\}_{t\geq 0}$ is a m-dimensional *Wiener process* (a.k.a. Brownian motion) defined on $(\Omega, \mathcal{F}, \pi)$. We write

$$\mathbf{W}(t) = (W^1(t), \ldots, W^m(t)).$$

(iii) $\mathbf{b} : \mathbb{R}^n \to \mathbb{R}^n$, $\mathbf{b} = (b_1, \ldots, b_n)$ and $\boldsymbol{B} : \mathbb{R}^n \to \mathbb{M}^{n\times m}$, $\boldsymbol{B} = ((b_{ij}))$ are given Lipschitz functions.

(iv) $\mathbf{X_0}$ is a $\mathbb{R}^n$-valued random variable defined on $(\Omega, \mathcal{F}, \pi)$.

(v) $\mathcal{F}(t) = \sigma(\mathbf{X_0}, \mathbf{W}(s)(0 \leq s \leq t))$, the smallest σ-algebra with respect to which $\mathbf{X_0}$ and $\mathbf{W}(s)$ for $0 \leq s \leq t$ are measurable. □

We intend to study the *stochastic differential equation*

$$(1) \qquad \begin{cases} d\mathbf{X}(t) &= \mathbf{b}(\mathbf{X}(t))dt + \boldsymbol{B}(\mathbf{X}(t))d\mathbf{W}(t) \qquad (t > 0) \\ \mathbf{X}(0) &= \mathbf{X_0} \end{cases}$$

for the unknown $\mathbb{R}^n$-valued stochastic process $\{\mathbf{X}(t)\}_{t\geq 0}$ defined on $(\Omega, \mathcal{F}, \pi)$.

Remarks. (i) We say $\{\mathbf{X}(t)\}_{t\geq 0}$ *solves* (1) provided this process is progressively measurable with respect to $\{\mathcal{F}_t\}_{t\geq 0}$ and

$$(2) \qquad \mathbf{X}(t) = \mathbf{X_0} + \int_0^t \mathbf{b}(\mathbf{X}(s))ds + \int_0^t \boldsymbol{B}(\mathbf{X}(s)) \cdot d\mathbf{W}(s)$$

a.s., for each time $t \geq 0$. The last term on the right is an *Itô stochastic integral*, defined for instance in [A], [FR], etc.

(ii) We may *heuristically* rewrite (1) to read

$$\begin{cases} \dot{\mathbf{X}}(t) &= \mathbf{b}(\mathbf{X}(t)) + \boldsymbol{B}(\mathbf{X}(t)) \cdot \boldsymbol{\xi}(t) \qquad (t \geq 0), \\ \mathbf{X}(0) &= \mathbf{X_0} \end{cases} \tag{3}$$

where $\cdot = \frac{d}{dt}$ and

$$\text{“}\boldsymbol{\xi}(t) = \frac{d\mathbf{W}(t)}{dt} = m\text{-dimensional } \textit{white noise}\text{.”} \tag{4}$$

(iii) If we additionally assume that $\mathbf{X_0}$ is independent of $\{\mathbf{W}(t)\}_{t\geq 0}$ and $E(|\mathbf{X_0}|^2) < \infty$, then there exists a unique solution $\{\mathbf{X}(t)\}_{t\geq 0}$ of (1), such that

$$E\left(\int_0^T |\mathbf{X}(t)|^2 dt\right) < \infty \tag{5}$$

for each time $T > 0$. “Unique” here means that if $\{\tilde{\mathbf{X}}(t)\}_{t\geq 0}$ is another process solving (1) and satisfying an estimate like (5), then

$$\pi(\mathbf{X}(t) = \tilde{\mathbf{X}}(t) \text{ for all } 0 \leq t \leq T) = 1 \tag{6}$$

for each $T > 0$. Furthermore, the sample paths $t \mapsto X(t)$ are continuous, with probability one.

2. Itô's formula, elliptic PDE

Solutions of (1) are connected to solutions of certain linear elliptic PDE of second order. The key is *Itô's chain rule*, which states that if $u : \mathbb{R}^n \to \mathbb{R}$ is a C^2-function, then

$$\begin{aligned} du(\mathbf{X}(t)) &= Du(\mathbf{X}(t)) \cdot d\mathbf{X}(t) \\ &+ \tfrac{1}{2}\mathbf{A}(\mathbf{X}(t)) : D^2u(\mathbf{X}(t))dt \qquad (t \geq 0), \end{aligned} \tag{7}$$

where $\mathbf{A} : \mathbb{R}^n \to \mathbb{M}^{n\times n}$ is defined by

$$\mathbf{A} = \boldsymbol{B}\boldsymbol{B}^T.$$

Remarks. (i) If we write $A = ((a^{ij}))$, then

$$\sum_{i,j=1}^n a^{ij}\xi_i\xi_j \geq 0 \qquad (\xi \in \mathbb{R}^n). \tag{8}$$

(ii) Formula (7) means

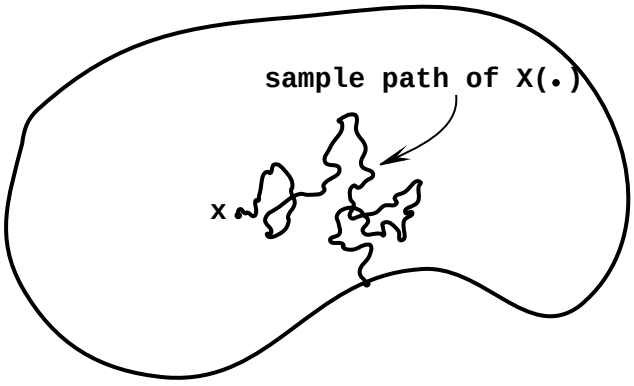
$$
\begin{aligned}
u(\mathbf{X}(t)) &= u(\mathbf{X}(0)) \\
&+ \int_0^t \sum_{i=1}^n b_i(\mathbf{X}(s)) u_{x_i}(\mathbf{X}(s)) + \tfrac{1}{2} \sum_{i,j=1}^n a^{ij}(\mathbf{X}(s)) u_{x_i x_j}(\mathbf{X}(s)) ds \\
&+ \int_0^t \sum_{i=1}^n \sum_{k=1}^m \theta_{ik}(\mathbf{X}(s)) u_{x_i}(\mathbf{X}(s)) dW^k(s)
\end{aligned} \tag{9}
$$

for each time $t \geq 0$. □

Next assume u solves the PDE[4]

$$
\begin{cases}
\frac{1}{2} \sum_{i,j=1}^n a^{ij} u_{x_i x_j} + \sum_{i=1}^n b_i u_{x_i} &= 0 \text{ in } U \\
u &= g \text{ on } \partial U,
\end{cases} \tag{10}
$$

where $U \subset \mathbb{R}^n$ is a bounded, connected open set with smooth boundary, and $g : \partial U \to \mathbb{R}$ is given. In view of (8) this is a (possibly degenerate) elliptic PDE.



Fix a point $x \in U$ and let $\{\mathbf{X}(t)\}_{t \geq 0}$ solve the stochastic DE

$$
\begin{cases}
d\mathbf{X}(t) = \mathbf{b}(\mathbf{X}(t)) dt + \boldsymbol{B}(\mathbf{X}(t)) d\mathbf{W}(t) \qquad (t > 0) \\
\mathbf{X}(0) = x.
\end{cases} \tag{11}
$$

Define also the *hitting time*

$$
\tau_x := \min\{t \geq 0 \mid \mathbf{X}(t) \in \partial U\}. \tag{12}
$$

Assume, as will be the case in §3,4 following, that $\tau_x < \infty$ a.s. We apply Itô's formula, with u a solution of (10) and the random variable τ_x replacing t:

$$
u(\mathbf{X}(\tau_x)) = u(\mathbf{X}(0)) + \int_0^{\tau_x} Du \cdot \boldsymbol{B}\, d\mathbf{W}.
$$

[4]Note that there is no minus sign in front of the term involving the second derivatives: this differs from the convention in [E1, Chapter VI].

But $\mathbf{X}(0) = x$ and $u(\mathbf{X}(\tau_x)) = g(\mathbf{X}(\tau_x))$. Thus

$$u(x) = g(\mathbf{X}(\tau_x)) - \int_0^{\tau_x} Du \cdot \boldsymbol{B}\, d\mathbf{W}.$$

We take expected values, and recall from [A], [FR], etc. that

$$E\left(\int_0^{\tau_x} Du \cdot \boldsymbol{B} d\mathbf{W}\right) = 0,$$

to deduce this *stochastic representation formula* for u:

$$u(x) = E(g(\mathbf{X}(\tau_x))) \qquad (x \in U). \tag{13}$$

Note that $\mathbf{X}$ and τ_x here depend on x.

3. An exit problem

We hereafter assume the uniform ellipticity condition

$$\sum_{i,j=1}^{n} a^{ij}(x)\xi_i\xi_j \geq \theta|\xi|^2 \tag{14}$$

and suppose also that b_i, a^{ij} $(1 \leq i, j \leq n)$ are smooth.

a. Small noise asymptotics

Take $\varepsilon > 0$. We rescale the noise term in (11):

$$\begin{cases} dX^\varepsilon(t) &= \mathbf{b}(\mathbf{X}^\varepsilon(t))dt + \varepsilon \boldsymbol{B}(\mathbf{X}^\varepsilon(t)) \cdot d\mathbf{W}(t) \qquad (t \geq 0) \\ \mathbf{X}^\varepsilon(0) &= x. \end{cases} \tag{15}$$

Now as $\varepsilon \to 0$, we can expect the random trajectories $t \mapsto \mathbf{X}^\varepsilon(t)$ to converge somehow to the deterministic trajectories $t \mapsto \mathbf{x}(t)$, where

$$\begin{cases} \dot{\mathbf{x}}(t) &= \mathbf{b}(\mathbf{x}(t)) \qquad (t \geq 0) \\ \mathbf{x}(0) &= x. \end{cases} \tag{16}$$

We are therefore interpreting (15) as modeling the dynamics of a particle moving with velocity $\mathbf{v} = \mathbf{b}$ plus a small noise term. What happens when $\varepsilon \to 0$?

This problem fits into the large deviations framework. We take $\Sigma = C([0,T];\mathbb{R}^m)$ for some $T > 0$ and write P_ε to denote the distribution of the process $\mathbf{X}^\varepsilon(\cdot)$ on Σ. Freidlin

and Wentzell have shown that $\{P_\varepsilon\}_{0<\varepsilon\leq 1}$ satisfying the large deviation principle with a rate function $I[\cdot]$, defined this way:

(17)
$$I[\mathbf{y}(\cdot)] = \begin{cases} \frac{1}{2}\int_0^T \sum_{i,j=1}^n a^{ij}(\mathbf{y}(s))(\dot{\mathbf{y}}_i(s) - b_i(\mathbf{y}(s)))(\dot{\mathbf{y}}_j(s) - b_j(\mathbf{y}(s)))ds & \text{if } \mathbf{y}(\cdot) \in H^1([0,T];\mathbb{R}^n) \\ +\infty & \text{otherwise.} \end{cases}$$

Here $((a^{ij})) = \mathbf{A}^{-1}$ is the inverse of the matrix $\mathbf{A} = \mathbf{D}\mathbf{D}^T$ and $H^1([0,T];\mathbb{R}^n)$ denotes the Sobolev space of mappings from $[0,T] \to \mathbb{R}^n$ which are absolutely continuous, with square integrable derivatives. We write $\mathbf{y}(\cdot) = (y_1(\cdot), \ldots, y_n(\cdot))$.

b. Perturbations against the flow

We present now a PDE method for deriving an interesting special case of the aforementioned large derivation result, and in particular demonstrate how $I[\cdot]$ above arises. We follow Fleming [FL] and [E-I].

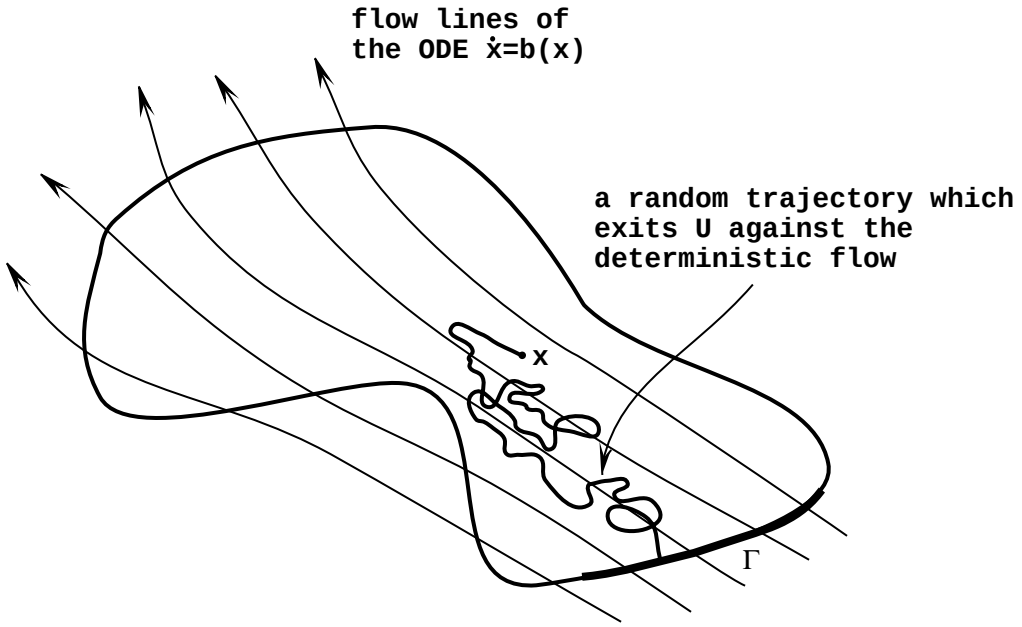
To set up this problem, take $U \subset \mathbb{R}^n$ as above, fix a point $x \in U$, and let $\{\mathbf{X}^\varepsilon(t)\}_{t\geq 0}$ solve the stochastic ODE (15). We now also select a smooth, relatively open subregion $\Gamma \subset \partial U$ and ask:

(18)
$$\begin{cases} \text{For small } \varepsilon > 0, \text{ what is the probability} \\ \text{that } \mathbf{X}^\varepsilon(t) \text{ first exits } U \text{ through the} \\ \text{region } \Gamma? \end{cases}$$

This is in general a very difficult problem, and so we turn attention to a special case, by hypothesizing concerning the vector field $\mathbf{b}$ that

(19)
$$\begin{cases} \text{if } \mathbf{y}(\cdot) \in H^1_{\text{loc}}([0,\infty);\mathbb{R}^n) \text{ and} \\ \mathbf{y}(t) \in U \text{ for all } t \geq 0, \text{ then} \\ \quad \int_0^\infty |\dot{\mathbf{y}}(t) - \mathbf{b}(\mathbf{y}(t))|^2 dt = +\infty. \end{cases}$$

Condition (19) says that it requires an infinite amount of "energy" for a curve $\mathbf{y}(\cdot)$ to resist being swept along with the flow $\mathbf{x}(\cdot)$ determined by $\mathbf{b}$, staying within U for all times $t \geq 0$.



Intuitively we expect that for small $\varepsilon > 0$, the overwhelming majority of the sample paths of $\mathbf{X}^\varepsilon(\cdot)$ will stay close to $\mathbf{x}(\cdot)$ and so be swept out of ∂U in finite time. If, on the other hand we take for Γ a smooth "window" within ∂U lying upstream from x, the probability that a sample path of $\mathbf{X}^\varepsilon(\cdot)$ will move against the flow and so exit U through Γ should be very small.

Notation. (i)

$$\begin{aligned} u^\varepsilon(x) &= \text{probability that } \mathbf{X}^\varepsilon(\cdot) \text{ first exits} \\ &\quad \partial U \text{ through } \Gamma \\ &= \pi(\mathbf{X}^\varepsilon(\tau_x) \in \Gamma). \end{aligned} \tag{20}$$

(ii)

$$g = \chi_\Gamma = \begin{cases} 1 & \text{on } \Gamma \\ 0 & \text{on } \partial U - \Gamma. \end{cases} \tag{21}$$

□

Then

$$u^\varepsilon(x) = E(g(\mathbf{X}^\varepsilon(\tau_x))) \qquad (x \in U). \tag{22}$$

But according to §b, $u^\varepsilon(\cdot)$ solves the boundary value problem

$$\begin{cases} \frac{\varepsilon^2}{2} \sum_{i,j=1}^n a^{ij} u^\varepsilon_{x_i x_j} + \sum_{i=1}^n b_i u^\varepsilon_{x_i} &= 0 \text{ in } U \\ u^\varepsilon &= 1 \text{ on } \Gamma \\ u^\varepsilon &= 0 \text{ on } \partial U - \bar{\Gamma}. \end{cases} \tag{23}$$

We are interested in the asymptotic behavior of the function u^ε as $\varepsilon \to 0$.

Theorem. *Assume U is connected. We then have*

$$u^\varepsilon(x) = e^{-\frac{w(x)+o(1)}{\varepsilon^2}} \qquad \text{as } \varepsilon \to 0, \tag{24}$$

uniformly on compact subsets of $U \cup \Gamma$, where

$$w(x) := \inf_{\mathcal{A}} \left\{ \frac{1}{2} \int_0^\tau \sum_{i,j=1}^n a^{ij}(\mathbf{y}(s))(\dot{\mathbf{y}}_i(s) - b_i(\mathbf{y}(s)))(\dot{\mathbf{y}}_j(s) - b_j(\mathbf{y}(s)))ds \right\}, \tag{25}$$

the infimum taken among curves in the admissible class

$$\mathcal{A} = \{\mathbf{y}(\cdot) \in H^1_{\text{loc}}([0,\infty);\mathbb{R}^n) \mid \mathbf{y}(t) \in U \text{ for } 0 \le t < \tau,\ \mathbf{y}(\tau) \in \Gamma \text{ if } \tau < \infty\}. \tag{26}$$

Proof (Outline). 1. We introduce a rescaled version of the log transform from Chapter IV, by setting

$$w^\varepsilon(x) := -\varepsilon^2 \log u^\varepsilon(x) \qquad (x \in U). \tag{27}$$

According to the Strong Maximum Principle,

$$0 < u^\varepsilon(x) < 1 \text{ in } U$$

and so the definition (27) makes sense, with

$$w^\varepsilon > 0 \text{ in } U.$$

We compute:

$$\begin{cases} w^\varepsilon_{x_i} &= -\varepsilon^2 \frac{u^\varepsilon_{x_i}}{u^\varepsilon}, \\ w^\varepsilon_{x_i x_j} &= -\varepsilon^2 \frac{u^\varepsilon_{x_i x_j}}{u^\varepsilon} + \varepsilon^2 \frac{u^\varepsilon_{x_i} u^\varepsilon_{x_j}}{(u^\varepsilon)^2}. \end{cases}$$

Thus our PDE (23) becomes

$$\begin{cases} -\frac{\varepsilon^2}{2} \sum_{i,j=1}^n a^{ij} w^\varepsilon_{x_i x_j} + \frac{1}{2} \sum_{i,j=1}^n a^{ij} w^\varepsilon_{x_i} w^\varepsilon_{x_j} - \sum_{i=1}^n b_i w^\varepsilon_{x_i} &= 0 \quad \text{in } U \\ w^\varepsilon &= 0 \quad \text{on } \Gamma \\ w^\varepsilon &\to \infty \quad \text{at } \partial U - \bar{\Gamma}. \end{cases} \tag{28}$$

2. We intend to estimate $|Dv^\varepsilon|$ on compact subsets of $U \cup \Gamma$, as in §IV.A.2. For this let us first differentiate PDE:

$$-\frac{\varepsilon^2}{2} \sum_{i,j=1}^n a^{ij} w^\varepsilon_{x_k x_i x_j} + \sum_{i,j=1}^n a^{ij} w^\varepsilon_{x_k x_i} w^\varepsilon_{x_j} - \sum_{i=1}^n b_i w^\varepsilon_{x_k x_i} = R_1, \tag{29}$$

where the remainder term R_1 satisfies the estimate

$$|R_1| \leq C(\varepsilon^2|D^2w^\varepsilon| + |Dw^\varepsilon|^2 + 1).$$

Now set

$$\gamma := |Dw^\varepsilon|^2, \tag{30}$$

so that

$$\left\{ \begin{array}{rcl} \gamma_{x_i} & = & 2\sum_{k=1}^n w^\varepsilon_{x_k} w^\varepsilon_{x_k x_i} \\ \gamma_{x_i x_j} & = & 2\sum_{k=1}^n w^\varepsilon_{x_k} w^\varepsilon_{x_k x_i x_j} + w^\varepsilon_{x_k x_i} w^\varepsilon_{x_k x_j}. \end{array} \right.$$

Thus

$$\begin{array}{l} -\frac{\varepsilon^2}{2}\sum_{i,j=1}^n a^{ij}\gamma_{x_i x_j} - \sum_{i=1}^n b_i \gamma_{x_i} \\ = 2\sum_{k=1}^n w^\varepsilon_{x_k}\left(-\frac{\varepsilon^2}{2}\sum_{i,j=1}^n a^{ij} w^\varepsilon_{x_k x_i x_j} - \sum_{i=1}^n b_i w^\varepsilon_{x_i x_j}\right) \\ -\varepsilon^2 \sum_{k=1}^n \sum_{i,j=1}^n a^{ij} w^\varepsilon_{x_k x_i} w^\varepsilon_{x_k x_j}. \end{array} \tag{31}$$

Now

$$\sum_{k=1}^n \sum_{i,j=1}^n a^{ij} w^\varepsilon_{x_k x_i} w^\varepsilon_{x_k x_j} \geq \theta |D^2 w^\varepsilon|^2.$$

This inequality and (29) imply:

$$-\frac{\varepsilon^2}{2}\sum_{i,j=1}^n a^{ij}\gamma_{x_i x_j} - \sum_{i=1}^n b_i \gamma_{x_i} \leq -\varepsilon^2\theta |D^2 w^\varepsilon|^2 + R_2, \tag{32}$$

where

$$\begin{array}{rcl} |R_2| & \leq & C(\varepsilon^2 |D^2 w^\varepsilon||Dw^\varepsilon| + |Dw^\varepsilon|^3 + 1) \\ & \leq & \frac{\varepsilon^2\theta}{2}|D^2 w^\varepsilon|^2 + C(|Dw^\varepsilon|^3 + 1) \\ & = & \frac{\varepsilon^2\theta}{2}|D^2 w^\varepsilon|^2 + C(\gamma^{3/2} + 1). \end{array}$$

Consequently (32) yields the inequality:

$$\frac{\theta\varepsilon^2}{2}|D^2 w^\varepsilon|^2 - \frac{\varepsilon^2}{2}\sum_{i,j=1}^n a^{ij}\gamma_{x_i x_j} - \sum_{i=1}^n b_i \gamma_{x_i} \leq C(\gamma^{3/2} + 1). \tag{33}$$

Now the PDE (28) implies

$$\begin{array}{rcl} \gamma & \leq & C(\varepsilon^2 |D^2 w^\varepsilon| + |Dw^\varepsilon|) \\ & = & C(\varepsilon^2 |D^2 w^\varepsilon| + \gamma^{1/2}) \\ & \leq & C(\varepsilon^2 |D^2 w^\varepsilon| + 1) + \frac{\gamma}{2}, \end{array}$$

and so

$$\gamma \le C(\varepsilon^2 |D^2 w^\varepsilon| + 1).$$

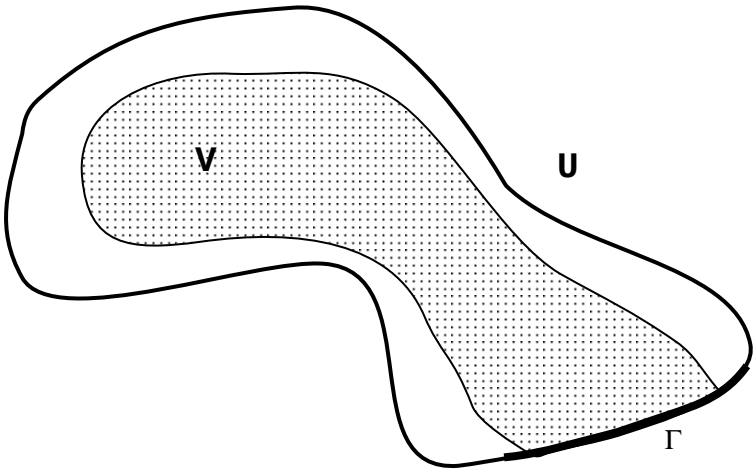
This inequality and (33) give us the estimate:

$$\sigma\gamma^2 - \frac{\varepsilon^4}{2}\sum_{i,j=1}^n a^{ij}\gamma_{x_i x_j} \le \varepsilon^2 C(|D\gamma| + \gamma^{3/2}) + C, \tag{34}$$

for some $\sigma > 0$.

3. We employ this differential inequality to estimate γ. Take any subregion $V \subset\subset U \cup \Gamma$ and select then a smooth cutoff function ζ such that

$$\begin{cases} 0 \le \zeta \le 1,\ \zeta \equiv 1 \text{ on } V, \\ \zeta \equiv 0 \text{ near } \partial U - \Gamma. \end{cases}$$



Write

$$\eta := \zeta^4 \gamma \tag{35}$$

and compute

$$\begin{cases} \eta_{x_i} &= \zeta^4 \gamma_{x_i} + 4\zeta^3 \zeta_{x_i} \gamma \\ \eta_{x_i x_j} &= \zeta^4 \gamma_{x_i x_j} + 4\zeta^3(\zeta_{x_j}\gamma_{x_i} + \zeta_{x_i}\gamma_{x_j}) + 4(\zeta^3 \zeta_{x_i})_{x_j}\gamma. \end{cases} \tag{36}$$

Select a point $x_0 \in \bar{U}$ where η attains its maximum. Consider first the case that $x_0 \in U$, $\zeta(x_0) > 0$. Then

$$D\eta(x_0) = 0,\ D^2\eta(x_0) \le 0.$$

Owing to (27)

$$\zeta D\gamma = -4\gamma D\zeta \text{ at } x_0, \tag{37}$$

and also

$$-\sum_{i,j=1}^{n} a^{ij}\eta_{x_i x_j} \geq 0 \text{ at } x_0.$$

Thus at x_0:

$$0 \leq -\frac{\varepsilon^4}{2}\sum_{i,j=1}^{n} a^{ij}\eta_{x_i x_j} = -\frac{\varepsilon^4}{2}\zeta^4 \sum_{i,j=1}^{n} a^{ij}\gamma_{x_i x_j} + R_3$$

where

$$\begin{aligned} |R_3| &\leq \varepsilon^4 C(\zeta^3|D\gamma| + \zeta^2\gamma) \\ &\leq \varepsilon^4 C\zeta^2\gamma. \end{aligned}$$

Therefore (25) implies

$$\begin{aligned} \sigma\zeta^4\gamma^2 &\leq \varepsilon^2\zeta^4 C(|D\gamma| + \gamma^{3/3}) + \varepsilon^4 C\zeta^2\gamma + C \\ &\leq \tfrac{\sigma\zeta^4}{2}\gamma^2 + C. \end{aligned}$$

Thus we can estimate $\eta = \zeta^4\gamma$ at x_0 and so bound $|Dw^\varepsilon(x_0)|$.

4. If on the other hand $x_0 \in \partial U$, $\zeta(x_0) > 0$, then we note $u^\varepsilon \equiv 1$ on ∂U near x_0. In this case we employ a standard barrier argument to obtain the estimate

$$|Du^\varepsilon(x_0)| \leq \frac{C}{\varepsilon^2},$$

from which it follows that

$$|Dw^\varepsilon(x_0)| = \varepsilon^2 \frac{|Du^\varepsilon(x_0)|}{u^\varepsilon(x_0)} \leq C. \tag{38}$$

Hence we can also estimate $\eta = \zeta^4\gamma = \zeta^4|Dw^\varepsilon|^2$ if $x_0 \in \partial U$. It follows that

$$\sup_V |Dw^\varepsilon| \leq C \tag{39}$$

for each $V \subset\subset U \cup \Gamma$, the constant C depending only on V and not on ε.

5. As $w^\varepsilon = 0$ on Γ, we deduce from (39) that

$$\sup_V |w^\varepsilon| \leq C. \tag{40}$$

In view of (39), (40) there exists a sequence $\varepsilon_r \to 0$ such that

$$\begin{cases} w^{\varepsilon_r} \to \tilde{w} \text{ uniformly on compact} \\ \text{subsets of } U \cup \Gamma. \end{cases}$$

It follows from (28) that

$$\tilde{w} = 0 \text{ on } \Gamma \tag{41}$$

and

$$\frac{1}{2}\sum_{i,j=1}^{n} a^{ij}\tilde{w}_{x_i}\tilde{w}_{x_j} - \sum_{i=1}^{n} b_i \tilde{w}_{x_i} = 0 \text{ in } U, \tag{42}$$

in the viscosity sense: the proof is a straightforward adaptation of the vanishing viscosity calculation in §VI.A. Since the PDE (42) holds a.e., we conclude that

$$|D\tilde{w}| \leq C \text{ a.e. in } U,$$

and so

$$\tilde{w} \in C^{0,1}(\bar{U}).$$

We must identify $\tilde{w}$.

6. For this, we recall the definition

$$w(x) = \inf_{\mathbf{y}(\cdot)\in\mathcal{A}} \left\{ \frac{1}{2}\int_0^\tau \sum_{i,j=1}^{n} a^{ij}(\mathbf{y}(s))(\dot{\mathbf{y}}_i(s) - b_i(\mathbf{y}(s)))(\dot{\mathbf{y}}_j(s) - b_j(\mathbf{y}(s)))ds \right\}, \tag{43}$$

the admissible class $\mathcal{A}$ defined by (26). Clearly then

$$w = 0 \text{ on } \Gamma. \tag{44}$$

We claim that in fact

$$\frac{1}{2}\sum_{i,j=1}^{n} a^{ij} w_{x_i} w_{x_j} - \sum_{i=1}^{n} b_i w_{x_i} = 0 \text{ in } U, \tag{45}$$

in the viscosity sense. To prove this, take a smooth function v and suppose

$$w - v \text{ has a local maximum at a point } x_0 \in U. \tag{46}$$

We must show

$$\frac{1}{2}\sum_{i,j=1}^{n} a^{ij} v_{x_i} v_{x_j} - \sum_{i=1}^{n} b_i v_{x_i} \leq 0 \text{ at } x_0. \tag{47}$$

To establish (47), note that (46) implies

$$w(x) - v(x) \leq w(x_0) - v(x_0) \text{ if } x \in B(x_0, r) \tag{48}$$

for r small enough.

Fix any $\alpha \in \mathbb{R}^n$ and consider the ODE

$$\begin{cases} \dot{\mathbf{y}}(s) &= \mathbf{b}(\mathbf{y}(s)) + A(\mathbf{y}(s))\alpha \qquad (s > 0) \\ \mathbf{y}(0) &= x_0. \end{cases} \tag{49}$$

Let $t > 0$ be so small that $\mathbf{y}(t) \in B(x_0, r)$. Then (43) implies

$$w(x_0) \leq \frac{1}{2} \int_0^t \sum_{i,j=1}^n a^{ij}(\mathbf{y}(s))(\dot{\mathbf{y}}_i - b_i(\mathbf{y}))(\dot{\mathbf{y}}_j - b_j(\mathbf{y}))ds + w(\mathbf{y}(t)).$$

Therefore (48), (49) give the inequality

$$\begin{aligned} v(x_0) - v(\mathbf{y}(t)) &\leq w(x_0) - w(\mathbf{y}(t)) \\ &\leq \tfrac{1}{2} \textstyle\int_0^t \sum_{i,j=1}^n a^{ij}(\mathbf{y}(s))\alpha_i\alpha_j ds. \end{aligned}$$

Divide by t and let $t \to 0$, recalling the ODE (49):

$$-Dv \cdot (b + A\alpha) \leq \frac{1}{2}(A\alpha) \cdot \alpha \text{ at } x_0.$$

This is true for all vectors $\alpha \in \mathbb{R}^n$, and consequently

$$\sup_{\alpha \in \mathbb{R}^n} \left(-Dv \cdot (b + A\alpha) - \frac{1}{2}(A\alpha) \cdot \alpha \right) \leq 0 \text{ at } x_0. \tag{50}$$

But the supremum above is attained for

$$\alpha = -Dv,$$

and so (50) says

$$\frac{1}{2}(ADv) \cdot Dv - b \cdot Dv \leq 0 \text{ at } x_0.$$

This is (47).

7. Next let us suppose

$$w - v \text{ has a local minimum at a point } x_0 \in U, \tag{51}$$

and prove

$$\frac{1}{2}\sum_{i,j=1}^{n} a^{ij} v_{x_i} v_{x_j} - \sum_{i=1}^{n} b_i v_{x_j} \geq 0 \text{ at } x_0. \tag{52}$$

To verify this inequality, we assume instead that (52) fails, in which case

$$\frac{1}{2}\sum_{i,j=1}^{n} a^{ij} v_{x_i} v_{x_j} - \sum_{i=1}^{n} b_i v_{x_i} \leq -\theta < 0 \text{ near } x_0 \tag{53}$$

for some constant $\theta > 0$. Now take a small time $t > 0$. Then the definition (43) implies that there exists $\mathbf{y}(\cdot) \in \mathcal{A}$ such that

$$w(x_0) \geq w(\mathbf{y}(t)) + \frac{1}{2}\int_0^t \sum_{i,j=1}^{n} a^{ij}(\mathbf{y})(\dot{\mathbf{y}}_i - b_i(\mathbf{y}))(\dot{\mathbf{y}}_j - b_j(\mathbf{y}))ds - \frac{\theta}{2}t.$$

In view of (51), therefore

$$\begin{array}{rcl} v(x_0) - v(\mathbf{y}(t)) & \geq & w(x_0) - w(\mathbf{y}(t)) \\ & \geq & \frac{1}{2}\int_0^t \sum_{i,j=1}^{n} a^{ij}(\mathbf{y})(\dot{\mathbf{y}}_i - b_i(\mathbf{y}))(\dot{\mathbf{y}}_j - b_j(\mathbf{y}))ds - \frac{\theta}{2}t. \end{array} \tag{54}$$

Now define

$$\alpha(s) := A^{-1}(\mathbf{y}(s))(\dot{\mathbf{y}} - \mathbf{b}(\mathbf{y}));$$

so that

$$\left\{ \begin{array}{rcl} \dot{\mathbf{y}}(s) & = & \mathbf{b}(\mathbf{y}(s)) + A(\mathbf{y}(s))\alpha(\mathbf{s}) \qquad (s > 0) \\ \mathbf{y}(0) & = & x_0. \end{array} \right. \tag{55}$$

Then

$$\begin{array}{rcl} v(x_0) - v(\mathbf{y}(t)) & = & -\int_0^t \frac{d}{ds} v(\mathbf{y}(s))ds \\ & = & -\int_0^t Dv(\mathbf{y}(s)) \cdot [\mathbf{b}(\mathbf{y}(s)) + A(\mathbf{y}(s))\alpha(\mathbf{s})]ds. \end{array}$$

Combine this identity with (54):

$$\begin{array}{rcl} -\frac{\theta}{2}t & \leq & \int_0^t (-Dv) \cdot (\mathbf{b}(\mathbf{y}) + A\boldsymbol{\alpha}(s)) - \frac{1}{2}(A\boldsymbol{\alpha}(s)) \cdot \boldsymbol{\alpha}(s))ds \\ & \leq & \int_0^t \sup_\alpha \left\{ (-Dv) \cdot (\mathbf{b}(\mathbf{y}) + A\alpha) - \frac{1}{2}(A\alpha) \cdot \alpha ds \right. \\ & = & \int_0^t \frac{1}{2}(ADv) \cdot Dv - \mathbf{b} \cdot Dv \; ds \\ & \leq & -\theta t, \end{array}$$

according to (53), provided $t > 0$ is small enough. This is a contradiction however.

We have verified (52).

8. To summarize, we have so far shown that $w^{\varepsilon_r} \to \tilde{w}$, $\tilde{w}$ solving the nonlinear first order PDE (42). Likewise w defined by (43) solves the same PDE. In addition $\tilde{w} = w = 0$ on Γ. We wish finally to prove that

$$\tilde{w} \equiv w \text{ in } U. \tag{56}$$

This is in fact true: the proof in [E-I] utilizes various viscosity solution tricks as well as the condition (19). We omit the details here.

Finally then, our main assertion (24) follows from (56). □

Appendix A: Units and constants

1. Fundamental quantities	**Units**
time	seconds (s)
length	meters (m)
mass	kilogram (kg)
temperature	Kelvin (K)
quantity	mole (mol)

2. Derived quantities	**Units**
force	$kg \cdot m \cdot s^{-2}$ = newton (N)
pressure	$N \cdot m^{-2}$ = pascal (Pa)
work, energy	$N \cdot m$ = joule (J)
power	$J \cdot s^{-1}$ = watt (W)
entropy	$J \cdot K^{-1}$
heat	4.1840 J = calorie

pressure = force/unit area

$$\text{work} = \begin{cases} \text{force} \times \text{distance} \\ \text{pressure} \times \text{volume} \end{cases}$$

power = rate of work

3. **Constants**

$R = \textit{gas constant} = 8.314\ J \cdot\ \text{mol}^{-1} \cdot K^{-1}$

$k = \textit{Boltzmann's constant} = 1.3806 \times 10^{-23}\ J \cdot K^{-1}$

$N_A = \textit{Avogadro's number} = R/k = 6.02 \times 10^{23}\ \text{mol}^{-1}$

Appendix B: Physical axioms

We record from Callen [C, p. 283-284] these physical "axioms" for a thermal system in equilibrium.

Postulate I. "There exist particular states (called equilibrium states) that, macroscopically, are characterized completely by the specification of the internal energy E and a set of extensive parameters $X_1, \ldots, X_m$, later to be specifically enumerated."

Postulate II. "There exists a function (called the entropy) of the extensive parameters, defined for all equilibrium states, and having the following property. The values assumed by the extensive parameters in the absence of a constraint are those that maximize the entropy over the manifold of constrained equilibrium states."

Postulate III. "The entropy of a composite system is additive over the constituent subsystems (whence the entropy of each constituent system is a homogeneous first-order function of the extensive parameters). The entropy is continuous and differentiable and is a monotonically increasing function of the energy."

Postulate IV. "The entropy of any system vanishes in the state for which $T = (\partial E/\partial S)_{X_1,\ldots,X_m} = 0$."

These statements are quoted verbatim, except for minor changes of notation. Postulate IV is the *Third Law* of thermodynamics, and is not included in our models.

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