I.1.3 Local thermodynamic equilibrium

In a more bottom-up approach to the modeling of a system Σ of discrete constituents as a continuous medium, one should first divide Σ (in thought) into small cells of fixed—yet not necessarily universal—size fulfilling two conditions:

(i) each individual cell can meaningfully be treated as a thermodynamic system, i.e. it must be large enough that the relative fluctuation of the usual extensive thermodynamic quantities computed for the content of the cell are negligible;

(ii) the thermodynamic properties vary little over the cell scale, i.e. cells cannot be too large, so that (approximate) homogeneity is ensured.

The rationale behind these two requirements is illustrated by Fig. I.1, which represents schematically how the value of a local macroscopic quantity, e.g. a density, depends on the resolution of the apparatus with which it is measured, i.e. equivalently on the length scale on which it is defined. If the apparatus probes too small a length scale, so that the discrete degrees of freedom become relevant, the measured value strongly fluctuates from one observation to the next one, as hinted at by the displayed envelope of possible results of measurements: this is the issue addressed by condition (i). Simultaneously, a small change in the measurement resolution, even with the apparatus still centered on the same point in the system, can lead to a large variation in the measured value of the observable, corresponding to the erratic behavior of the curve at small scales shown in Fig. I.1. This fluctuating pattern decreases with increasing size of the observation scale, since this increase leads to a growth in the number of atoms inside the probed volume, and thus a drop in the size of relative fluctuations. At the other end of the curve, one reaches a regime where the low resolution of the observation leads to encompassing domains with enough atoms to be rid of fluctuations, yet with inhomogeneous macroscopic properties, in a single probed region—in violation of condition (ii). As a result, the measured value of the density under consideration slowly evolves with the observation scale.

In between these two domains of strong statistical fluctuations and slow macroscopic variations lies a regime where the value measured for an observable barely depends on the scale over which it is

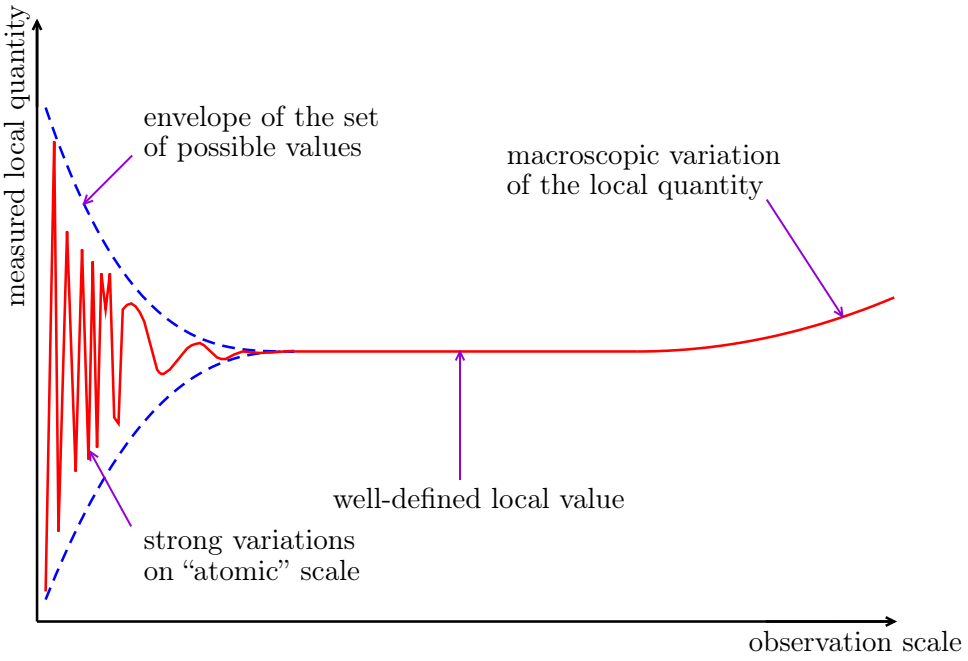

Figure I.1 – Typical variation of the measured value for a “local” macroscopic observable as a function of the size scale over which it is determined.

determined. This represents the appropriate regime for meaningfully defining—and measuring—a local density, and more general local quantities.

It is important to note that this intermediate "mesoscopic" interval may not always exist. There are physical systems in which strong macroscopic variations are already present in a range of scales where microscopic fluctuations are still sizable. For such systems, one cannot find scale-independent local variables. That is, the proper definition of local quantities implicitly relies on the existence of a clear separation of scales in the physical system under consideration, which is what will be assumed in the remainder of these notes.

Remark: The smallest volume over which meaningful local quantities can be defined is sometimes called *representative volume element*[(vii)] (RVE), or *representative elementary volume*.

When conditions (i) and (ii) hold, one may in particular define *local thermodynamic variables*, corresponding to the values taken in each intermediate-size cell—labeled by its position $\vec{r}$—by the usual extensive parameters: internal energy, number of atoms... Since the separation between cells is immaterial, nothing prevents energy or matter from being transported from a cell to its neighbors, even if the global system is isolated. Accordingly, the local extensive variables in any given cell are actually time-dependent in the general case. In addition, it becomes important to add linear momentum—with respect to some reference frame—to the set of local extensive variables characterizing the content of a cell.

The size of each cell is physically irrelevant, as long as it satisfies the two key requirements; there is thus no meaningful local variable corresponding to volume. Similarly, the values of the extensive variables in a given cell, which are by definition proportional to the cell size, are as arbitrary as the latter. They are thus conveniently replaced by the respective local densities: internal energy density $e(t,\vec{r})$, number density $n(t,\vec{r})$, linear momentum density $\rho(t,\vec{r})\,\vec{\mathrm{v}}(t,\vec{r})$, where ρ denotes the mass density, entropy density $s(t,\vec{r})$...

Remark: Rather than considering the densities of extensive quantities, some authors—in particular Landau & Lifshitz [3, 4]—prefer to work with *specific quantities*, i.e. their respective amounts per unit mass, instead of per unit volume. The relation between densities and specific quantities is trivial: denoting by $\mathcal{X}_j$ resp. $\mathcal{X}_{j,\mathrm{m}}$ a generic local density resp. specific amount for the same physical quantity, one has the identity

$$\mathcal{X}_j(t,\vec{r}) = \rho(t,\vec{r})\,\mathcal{X}_{j,\mathrm{m}}(t,\vec{r}) \tag{I.1}$$

in every cell—labeled by $\vec{r}$—and at every time t.

Once the local extensive variables have been meaningfully defined, one can develop the usual formalism of thermodynamics in each cell. In particular, one introduces the conjugate intensive variables, as e.g. local temperature $T(t,\vec{r})$ and pressure $\mathcal{P}(t,\vec{r})$. The underlying, important hypothesis is the assumption of a *local thermodynamic equilibrium*. According to the latter, the equation(s) of state of the system inside the small cell, expressed with local thermodynamic quantities, is the same as for a macroscopic system in the actual thermodynamic limit of infinitely large volume and particle number.

Consider for instance an non-relativistic classical ideal gas: its (mechanical) equation of state reads $\mathcal{P}\mathcal{V} = Nk_{\mathrm{B}}T$, with N the number of atoms, which occupy a volume $\mathcal{V}$ at uniform pressure $\mathcal{P}$ and temperature T, while k_{B} is the Boltzmann constant. This is trivially recast as $\mathcal{P} = nk_{\mathrm{B}}T$, with n the number density of atoms. The local thermodynamic equilibrium assumption then states that under non-uniform conditions of temperature and pressure, the equation of state in a local cell at position $\vec{r}$ is given by

$$\mathcal{P}(t,\vec{r}) = n(t,\vec{r})k_{\mathrm{B}}T(t,\vec{r}) \tag{I.2}$$

at every time t.

[(vii)] *Repräsentatives Volumen-Element*

The last step towards the continuous-medium model is to promote $\vec{r}$, which till now was simply the discrete label attached to a given cell, to be a continuous variable taking its values in $\mathbb{R}^3$—or rather, in the volume $\mathcal{V}_t$ attached to the system at the corresponding instant t. Accordingly, taking into account the time-dependence of physical quantities, the local variables, in particular the thermodynamic parameters, become *fields* on $\mathbb{R} \times \mathbb{R}^3$.

The replacement of the fine-resolution description, in which atoms are the relevant degrees of freedom, by the lower-resolution model which assimilates small finite volumes of the former to structureless points is called *coarse graining*[(viii)].

> This is a quite generic procedure in theoretical physics, whereby the finer degrees of freedom of a more fundamental description are smoothed away—technically, this is often done by performing averages or integrals, so that these degrees of freedom are "integrated out"—and replaced by novel, effective variables in a theory with a more limited range of applicability, but which is more tractable for "long-range" phenomena.

Coming back to condition (ii), we already stated that it implicitly involves the existence of at least one large length scale L, over which the macroscopic physical properties of the system may vary. This scale can be a characteristic dimension of the system under consideration, as e.g. the diameter of the tube in which a liquid is flowing. In the case of periodic waves propagating in the continuous medium, L also corresponds to their wavelength. More generally, if $\mathcal{G}$ denotes a macroscopic physical quantity, one may consider

$$L \cong \left[\frac{\left| \vec{\nabla} \mathcal{G}(t, \vec{r}) \right|}{\left| \mathcal{G}(t, \vec{r}) \right|} \right]^{-1}, \tag{I.3}$$

where $\vec{\nabla}$ denotes the (spatial) gradient.

Condition (i) in particular implies that the typical size of the cells which are later coarse grained should be significantly larger than the *mean free path* ℓ_{mfp} of atoms, so that thermodynamic equilibrium holds in the local cells. Since on the other hand this same typical size should be significantly smaller than the scale L of macroscopic variations, one deduces the condition

$$\mathrm{Kn} \equiv \frac{\ell_{\mathrm{mfp}}}{L} \ll 1 \tag{I.4}$$

on the dimensionless *Knudsen number* Kn.[(a)]

In air under normal conditions $\mathcal{P} = 10^5$ Pa and $T = 300$ K, the mean free path is $\ell_{\mathrm{mfp}} \approx 0.1$ μm. In the study of phenomena with variations on a characteristic scale $L \approx 10$ cm, one finds $\mathrm{Kn} \approx 10^{-6}$, so that air can be meaningfully treated as a continuous gas.

> The opposite regime $\mathrm{Kn} > 1$ is that of a *rarefied medium*, as for instance of the so-called Knudsen gas, in which the collisions between atoms are negligible—and in particular insufficient to ensure thermal equilibrium as an ideal gas. The flow of such systems is not well described by hydrodynamics, but necessitates alternative descriptions like molecular dynamics, in which the degrees of freedom are explicitly atoms.

I.2 Lagrangian description

The *Lagrangian*[(b)] perspective, which generalizes the approach usually adopted in the description of the motion of a (few) point particle(s), focuses on the trajectories of the material points, where the latter are labeled by their position in the reference configuration. Accordingly, physical quantities are expressed as functions of time t and initial position vectors $\vec{R}$, and any continuity condition has to be formulated with respect to these variables.

(viii) *Vergröberung*

(a) M. Knudsen, 1871-1949 (b) J.-L. Lagrange, 1736–1813

I.2.1 Lagrangian coordinates

Consider a material point M in a continuous medium. Given a reference frame $\mathcal{R}$, which allows the definition of its position vector at any time t, one can follow its *trajectory* $\vec{r}(t)$, which, after having chosen a coordinate system, is equivalently represented by the $\{x^i(t)\}$ for $i = 1, 2, 3$.

Let $\vec{R}$ resp. $\{X^i\}$ denote the position resp. coordinates of the material point M at t_0. The trajectory obviously depends on this "initial" position, and $\vec{r}$ can thus be viewed as a function of t and $\vec{R}$, where the latter refers to the reference configuration κ_0:

$$\vec{r} = \vec{r}(t, \vec{R}) \tag{I.5a}$$

with the consistency condition

$$\vec{r}(t{=}t_0, \vec{R}) = \vec{R}. \tag{I.5b}$$

In the *Lagrangian description*, also referred to as *material description* or *particle description*, this point of view is generalized, and the various physical quantities $\mathcal{G}$ characterizing a continuous medium are viewed at *any* time as mathematical functions of the variables t and $\vec{R}$:

$$\mathcal{G} = \mathcal{G}(t, \vec{R}), \tag{I.6}$$

where the mapping $\mathcal{G}$—which as often in physics will be denoted with the same notation as the physical quantity represented by its value—is defined for every t on the initial volume $\mathcal{V}_0$ occupied by the reference configuration κ_0.

Together with the time t, the position vector $\vec{R}$—or equivalently its coordinates X^1, X^2, X^3 in a given system—are called *Lagrangian coordinates*.

I.2.2 Continuity assumptions

An important example of physical quantity, function of t and $\vec{R}$, is simply the (vector) position in the reference frame $\mathcal{R}$ of material points at time t, i.e. $\vec{r}$ or equivalently its coordinates $\{x^i\}$, as given by relation (I.5a), which thus relates the configurations κ_0 and κ_t.

More precisely, $\vec{r}(t, \vec{R})$ maps for every t the initial volume $\mathcal{V}_0$ *onto* $\mathcal{V}_t$. To implement mathematically the physical picture of continuity, it will be assumed that the mapping $\vec{r}(t, \cdot) : \mathcal{V}_0 \to \mathcal{V}_t$ is also one-to-one for every t—i.e. all in all bijective—, and that the function $\vec{r}$ and its inverse

$$\vec{R} = \vec{R}(t, \vec{r}) \tag{I.7}$$

are *continuous* with respect to both time and space variables. This requirement in particular ensures that neighboring points remain close to each other as time elapses. It also preserves the connectedness of volumes, (closed) surfaces or curves along the evolution: one may then define *material domains*, i.e. connected sets of material points which are transported together in the evolution of the continuous medium.

For the sake of simplicity, it will be assumed that the mapping $\vec{r}$ and its inverse, and more generally every mathematical function $\mathcal{G}$ representing a physical quantity, is at least twice continuously differentiable (i.e. of class $\mathscr{C}^2$). To be able to accommodate for important phenomena that are better modeled with discontinuities, like shock waves in fluids (Sec. ???) or ruptures in solids—for instance, in the Earth's crust—, the $\mathscr{C}^2$-character of functions under consideration may only hold piecewise.

I.2.3 Velocity and acceleration of a material point

As mentioned above, for a fixed reference position $\vec{R}$ the function $t \mapsto \vec{r}(t, \vec{R})$ is the trajectory of the material point which passes through $\vec{R}$ at the reference time t_0. As a consequence, the velocity in the reference frame $\mathcal{R}$ of this same material point at time t is simply

$$\vec{v}(t, \vec{R}) = \frac{\partial \vec{r}(t, \vec{R})}{\partial t}. \tag{I.8}$$

Since the variable $\vec{R}$ is independent of t, one could actually also write $\vec{v}(t,\vec{R}) = \mathrm{d}\vec{r}(t,\vec{R})/\mathrm{d}t$. In turn, the acceleration of the material point in $\mathcal{R}$ is given at time t by

$$\vec{a}(t,\vec{R}) = \frac{\partial \vec{v}(t,\vec{R})}{\partial t}. \tag{I.9}$$

Remark: The trajectory (or *pathline*[ix]) of a material point can be visualized, by tagging the point at time t_0 at its position $\vec{R}$, for instance with a fluorescent or radioactive marker, and then imaging the positions at later times $t > t_0$.

If on the other hand one regularly—say for every instant $t_0 \leq t' \leq t$—injects some marker at a fixed geometrical point P, the resulting tagged curve at time t is the locus of the geometrical points occupied by medium particles which passed through P in the past. This locus is referred to as *streakline*.[x] Denoting by $\vec{r}_P$ the position vector of point P, the streakline is the set of geometrical points with position vectors

$$\vec{r} = \vec{r}\big(t, \vec{R}(t', \vec{r}_P)\big) \quad \text{for } t_0 \leq t' \leq t. \tag{I.10}$$

[ix] *Bahnlinie* [x] *Streichlinie*