

Chapter 11

Boltzmannian Non-Equilibrium and Local Variables



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Abstract Boltzmannian statistical mechanics (BSM) partitions a system's space of micro-states into cells and refers to these cells as 'macro-states'. One of these cells is singled out as the equilibrium macro-state while the others are non-equilibrium macro-states. It remains unclear, however, how these states are characterised at the macro-level as long as only real-valued macro-variables are available. We argue that physical quantities like pressure and temperature should be treated as field-variables and show how field variables fit into the framework of our own version of BSM, the long-run residence time account of BSM. The introduction of field variables into the theory makes it possible to give a full macroscopic characterisation of the approach to equilibrium.

11.1 Introduction

The central posit of Boltzmannian statistical mechanics (BSM) is that macro-states supervene on micro-states.¹ This leads to a partitioning of the state space of a system into regions of micro-states that are macroscopically indistinguishable, so-called macro-regions. How are macro-states defined and how are the corresponding macro-regions constructed? The standard answer, which goes back to Boltzmann's seminal (1877), is that macro-regions are constructed with what is now called

¹ This paper discusses BSM. For discussion of Gibbsian statistical mechanics see Frigg and Werndl (2021), and for a discussion of the relation between BSM and Gibbsian statistical mechanics see Werndl and Frigg (2017b) and Frigg and Werndl (2019).

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the combinatorial argument, and the largest macro-region is singled out as the equilibrium macro-region.²

This argument had considerable successes, most notably that it can establish the Maxwell-Boltzmann distribution as the equilibrium distribution of a dilute gas. At the same time it faces technical limitations and conceptual problems.³ An important formal limitation is that the argument only applies to systems consisting of non-interacting particles. Such systems are only a small subset of the systems BSM is interested in because the constituents of most systems *do* interact. Even if this technical limitation could be overcome somehow, one would be left with the conceptual quandary of why equilibrium is the state with the largest macro-region. The connection is not conceptual: there is nothing in the concept of equilibrium tying equilibrium to the largest macro-region. But if the connection is not conceptual, what justifies this association?

To solve these problems, we pursued the project of rethinking Boltzmannian equilibrium and proposed an alternative version of BSM (Werndl and Frigg, 2015a,b). While previous approaches often operated ‘bottom up’ in that they sought to define macro-states and equilibrium in terms of micro-mechanical properties, our approach works ‘top down’ in that it defines the macro-states and equilibrium in macroscopic terms. For reasons that will become clear soon, we call this the *long-run residence time account of BSM* (LBSM). Discussion of this account have hitherto focussed on real-valued macro-variables, i.e. macro-variables that assign a real number to every micro-state. This, however, leaves open how we should think about situations, where the system’s macro-state cannot be adequately described by a finite number of real-valued macro-variables. In this paper we take the next step and explicate how our account deals with such situations by using local variables.

The limitations of real-valued macro-variables become palpable in non-equilibrium situations. As an illustration, consider the expanding gas, an example that has become standard in foundational discussions of BSM. Imagine a gas confined to the left half of a container by a partition wall. When the partition wall is removed, the gas starts spreading and eventually fills the entire container uniformly. Once the gas fills the container uniformly, it is in equilibrium and its macro-state is specified by specific values of the gas’ pressure p , temperature T and volume V . The relation between these variables is then given by the Boyle-Charles law, which says that $pV = cT$, where c is a constant. This is possible because these variables assume the same values *everywhere* in the system: in equilibrium, the pressure in the top left corner of the container is the same as the pressure in the bottom right corner, and, indeed, the same as the pressure in every other place in the container. This allows us to assign the gas a single value for pressure and regard this value the pressure of the gas. This is not possible during the system’s *approach* to equilibrium. A split second after the partition wall has been removed, there is no

² Contemporary discussions of this argument can be found in Albert (2000, Ch. 3), Frigg (2008, Sec. 2), and Uffink (2007, Sec. 4).

³ For a discussion of these see Uffink’s (2007, Sec. 4) and Werndl and Frigg’s (2015a; 2015b).

such thing ‘the’ pressure of the gas. The value of the pressure in the leftmost parts of the container is still almost the same as before the removal of the wall; the value of the pressure in the rightmost parts of the container is still almost zero; and the value of pressure in the middle of the container is somewhere in-between the two. Real-valued macro-variables cannot capture this situation.⁴ Pressure is now a *field* that takes a value at every point in the container, and to describe the gas’ macro-state a split second after the removal of the wall, one has to specify the pressure field throughout the container.

Rather than describing situations like the expanding gas using fields, thermodynamics deems quantities like pressure undefined in such situations. This purism comes at a high price: the restriction of the scope of thermodynamics to systems in equilibrium. There are three reasons why BSM neither can nor should afford such rigour. First, it has always been one of the main aims of BSM to understand not only equilibrium, but also the *approach* to equilibrium. This requires that the relevant physical quantities are defined also in non-equilibrium situations so that we can trace their time evolution as the system approaches equilibrium. This is impossible if the relevant quantities are simply undefined outside equilibrium.

Second, BSM, as standardly presented, often starts by introducing a partition on the state space, calls the cells of the partition ‘macro-states’, and then singles out one of the cells (usually the largest) as the equilibrium macro-state.⁵ Since equilibrium is unique, it follows that all other macro-states are non-equilibrium macro-states. So BSM in fact always introduces non-equilibrium macro-states together with the equilibrium state. However, calling cells of a partition ‘macro-states’ lacks motivation (if not legitimacy) as long as no characterisation of these states in terms of macro-variables is available. If cells of a partition are to be macro-stated in more than just name, BSM will have to give a proper macro characterisation of them.

Third, thermodynamics’ rigour is out of sync with experimental practice, where quantities like pressure and temperature are measured, and assigned values, even when the system is not in equilibrium. If pressure measurements were performed on a system in a non-equilibrium state like the one that the system is in a short moment after the removal of the partition wall, one would find that the pressure varies considerably between different locations in the container with values in the leftmost parts still being almost the same as before the removal of the wall and values in the rightmost parts still being almost zero. But, on pain of incoherence, one cannot both make such measures and maintain that the quantities measured are undefined. The message we ought to take away from this example is not that pressure is undefined in non-equilibrium situations (and that talk of pressure is meaningless). The message is that the formalism needs to be developed so that it accommodates variables like local pressure.

To account for situations like the expanding gas we need field variables. The project for this paper is to show that LBSM, as formulated in our 2015 papers,

⁴ At least if one thinks that local pressure is defined at every point in space.

⁵ See, for instance, Goldstein (2001).

can accommodate such variables and to spell out the details. The result of this will be a fully general definition of macro-states that covers both equilibrium and non-equilibrium situations. To this end we first introduce LBSM, state some of its core results, and highlight the limitations of the current formulation (Sect. 11.2). We then distinguish between global and local physical quantities and explicate how local quantities can be accommodated in LBSM through scalar fields (Sect. 11.3). Formal definitions are only useful if they can be applied to relevant cases. We therefore discuss typical local variables like pressure and show explicitly how they can be defined in our framework (Sect. 11.4). We end with a conclusion (Sect. 11.5).

11.2 The Long-Run Residence Time Account of BSM

Statistical mechanics studies physical systems like a gas in a container, a magnet on a laboratory table and a liquid in a jar. Described mathematically, these systems have the structure of a *measure-preserving dynamical system*, i.e. a quadruple $(X, \Sigma_X, \phi_t, \mu)$.⁶ X is the state space of the system, i.e. a set containing all possible micro-states the system can be in. For a gas with n molecules X has $6n$ dimensions: three dimensions for the position of each particle and three dimensions for the momentum of each particle. Σ_X is a σ -algebra on X and μ is a measure on (X, Σ_X) , which is required to be invariant under the dynamics: $\mu_X(T_t(A)) = \mu_X(A)$ for all $A \in \Sigma_X$ and all t . The dynamics of the model is given by an *evolution function* $\phi_t : X \rightarrow X$, where $t \in \mathbb{R}$ if time is continuous and $t \in \mathbb{Z}$ if time is discrete. ϕ_t is assumed to be measurable in (t, x) and to satisfy the requirement $T_{t_1+t_2}(x) = T_{t_2}(T_{t_1}(x))$ for all $x \in X$ and all $t_1, t_2 \in \mathbb{R}$ or \mathbb{Z} . If, at a certain point of time t_0 , the system is in micro-state x_0 , then it will be in state $\phi_t(x_0)$ at a later time t . For systems that are governed by an equation of motion such as Newton's equation, ϕ_t corresponds to the solutions of this equation. The *trajectory* through a point x in X is the function $s_x : \mathbb{R} \rightarrow X$, $s_x(t) = T_t(x)$ (and *mutatis mutandis* for discrete time).

At the macro-level the system is characterised by a set of l *macro-variables* (for some $l \in \mathbb{N}$). From a mathematical point of view, macro-variables are measurable functions from X into another space \mathbb{V} . That is $v_i : X \rightarrow \mathbb{V}_i, x \mapsto v_i(x)$, $i = 1, \dots, l$. For example, if v_1 is the magnetisation of the system and the system is in micro-state x , then $v_1(x)$ is the magnetisation of the system when it is in micro-state x . It is important to note that the \mathbb{V}_i can be different for different i . For many of the standard macro-variables the space \mathbb{V}_i is \mathbb{R} because the variables take values in the real numbers. Examples for such macro-variables are internal energy and total magnetisation. For ease of presentation, we restrict our discussion to such variables

⁶ The presentation of LBSM follows Werndl and Frigg (2015b). This paper focuses on deterministic systems. The generalisation to stochastic classical systems is spelled out in Werndl and Frigg (2017a), where statements of the relevant definitions and results can be found.

in the remainder of this section. It is important, however, to be clear that there is no assumption that *all* \mathbb{V}_i have to be \mathbb{R} . In fact, \mathbb{V}_i can be any space. And this is more than just a mathematical possibility. In the next section we will exploit this flexibility and consider cases in which the \mathbb{V}_i are function spaces, which is precisely what we need to accommodate field variables.

A macro-state is defined by the *values* of a set of macro-variables $\{v_1, \dots, v_l\}$. We use capital letters V_i to denote the values of v_i and write $v_i(x) = V_i$ to express that variable v_i assumes value V_i when the system is in micro-state x . A macro-state is then defined by a particular set of values $\{V_1, \dots, V_l\}$. That is, the system is in macro-state M_{V_1, \dots, V_l} iff $v_1 = V_1, \dots, v_l = V_l$. In cases where values are real numbers, exact values can sometimes be unsuitable to define macro-states. In such case one can also define macro-states by the macro-variables taking values in a certain interval. One can then say that the model is in macro-state $M_{[A_1, B_1], \dots, [A_l, B_l]}$ iff $V_1 \in [A_1, B_1], \dots, V_l \in [A_l, B_l]$ for suitably chosen intervals. Such a move can be useful, for instance, if one wants to take the finite measurement precision of the available laboratory equipment into account. If the macro-states were defined by exact values, but an experiment would not be able to ever give an exact value, we would have to conclude that it is impossible to determine experimentally in which macro-state the system is. This would be unfortunate because macro-states were initially designed to allow physicists to give a description of the system at the macro-level. This problem can be circumvented by defining macro-states through intervals that are chosen in way that takes the precision of the available equipment into account.

Since macro-states *supervene* on micro-states, a system's micro-state uniquely determines its macro-state. This determination relation is normally many-to-one. Therefore, every macro-state M is associated with a *macro-region* X_M consisting of all micro-states for which the system is in M . For a complete set of macro-states the macro-regions form a partition of X (i.e. the different X_M do not overlap and jointly cover X). A set of macro-states is complete if it contains all macro-states that the system can possibly be in. The set can be 'too large' in the sense that it can contain states that the system never assumes; there can, however, be no states the system can be in that is not contained in the set.

One of these macro-states is the equilibrium macro-state of the system. Intuitively speaking, a system is in equilibrium when its properties do not change. This intuition is built into thermodynamics, where a system is said to be in equilibrium when all change has come to a halt and the thermodynamic properties of the system remain constant over time (Fermi, 2000, 4).⁷ However, such a definition of equilibrium cannot be implemented in BSM because measure-preserving dynamical systems exhibit Poincaré recurrence and time reversal invariance. As a consequence,

⁷ Being in thermodynamic equilibrium is an intrinsic property of the system, which offers a notion of 'internal equilibrium' (Guggenheim, 1967, 7). It contrasts with 'mutual equilibrium' (*ibid.*, 8), which is the relational property of *being in equilibrium with each other* that two systems eventually reach after being put into thermal contact with each other. When defining equilibrium in BSM it is the internal equilibrium that we are interested in.

when the time evolution of a system unfolds without outside influence, the system will eventually return arbitrarily close to the micro-state in which it started. Hence a system starting outside equilibrium (for instance, when the gas was confined to one half of the container) will eventually return to that macro-state. So in BSM no system will remain in any state forever.

This precludes a definition of equilibrium as the state which the system never leaves once it has reached it. The long-run residence time account of BSM aims to stay as close to the thermodynamic definition of equilibrium as the mathematical constraints imposed by measure-preserving dynamical systems permit, and, intuitively, defines equilibrium as the macro-state in which the system spends most of its time in the long run. To give a formal definition, we first have to introduce the concept of the long-run fraction of time $LF_A(x)$ that a system, which is in initial state x at time $t = 0$, spends in a subset A of X :⁸

$$LF_A(x) = \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t 1_A(T_\tau(x)) d\tau, \quad (11.1)$$

where $1_A(x)$ is the characteristic function of A : $1_A(x) = 1$ for $x \in A$ and 0 otherwise. Note that long-run fractions depend on the initial condition.

The notion of ‘most of its time’ can be read in two different ways, giving rise to two different notions of equilibrium. The first introduces a lower bound of $1/2$ for the fraction of time and stipulates that whenever a system spends more than half of the time in a particular macro-state, this state is the equilibrium state. Mathematically, let α be a real number in $(\frac{1}{2}, 1]$, and let ε be a very small positive real number. If there is a macro-state $M_{V_1^*, \dots, V_l^*}$ satisfying the following condition, then that state is the system’s α - ε -equilibrium state:

There exists a set $Y \subseteq X$ such that $\mu_X(Y) \geq 1 - \varepsilon$, and all initial states $x \in Y$ satisfy $LF_{X_{M_{V_1^*, \dots, V_l^*}}}(x) \geq \alpha$. A system is in equilibrium at time t iff its micro-state at t , x_t , is in $X_{M_{V_1^*, \dots, V_l^*}}$.

According to the second reading, ‘most of its time’ refers to the fact that the system spends more time in the equilibrium state than in any other state (and this can be less than 50% of its time). Mathematically, let γ be a real number in $(0, 1]$ and let ε be a very small positive real number. If there is a macro-state $M_{V_1^*, \dots, V_l^*}$ satisfying the following condition, then that state is the system’s γ - ε -equilibrium state:

There exists a set $Y \subseteq X$ such that $\mu_X(Y) \geq 1 - \varepsilon$ and for all initial conditions $x \in Y$: $LF_{X_{M_{V_1^*, \dots, V_l^*}}}(x) \geq LF_{X_M}(x) + \gamma$ for all macro-states $M \neq M_{V_1^*, \dots, V_l^*}$. Again, a system is in equilibrium at time t iff its micro-state at t , x_t , is in $X_{M_{V_1^*, \dots, V_l^*}}$.

⁸ We state the definitions for continuous time. The corresponding definitions for discrete time are obtained by replacing the integrals by sums.

It should come as no surprise that these two notions are not equivalent. More specifically, an α - ε -equilibrium is strictly stronger than a γ - ε -equilibrium in the sense that the existence of the former implies the existence of the latter but not vice versa.

These definitions are about the *time* a model spends in the equilibrium state. In contrast to the traditional version of BSM, LBSM does *not* define equilibrium in terms of a macro-region's size. For this reason it is not immediately clear what the two definitions of equilibrium imply about the *size* of the relevant equilibrium macro-regions. It is therefore a result of some importance that the equilibrium regions of α - ε -equilibrium states and of γ - ε -equilibrium states eventually turn out to be the largest macro-regions. So LBSM recovers the standard approach's dictum that equilibrium macro-states are ones with the largest macro-region, but it does not use this as a *definition* of equilibrium (thus avoiding the problem that such a definition is unmotivated), and it does not have to impose any restrictions on the interactions in the system because it eschews appeal to combinatorial considerations (thus avoiding the unwelcome consequence that BSM can only deal with non-interacting systems).

The relevant technical results are as follows. We call a macro-region β -*dominant* if its measure is greater or equal to β for a particular $\beta \in (\frac{1}{2}, 1]$, and we call a macro-region δ -*prevalent* if its measure is larger than the measure of any other macro-region by a margin of at least $\delta > 0$. One can then prove the following theorems (Werndl and Frigg, 2015b):

Dominance Theorem: If $M_{\alpha-\varepsilon-\text{eq}}$ is an α - ε -equilibrium, then the following holds for $\beta = \alpha(1 - \varepsilon)$: $\mu_X(X_{M_{\alpha-\varepsilon-\text{eq}}}) \geq \beta$.⁹

Prevalence Theorem: If $M_{\gamma-\varepsilon-\text{eq}}$ is a γ - ε -equilibrium, then the following holds for $\delta = \gamma - \varepsilon$: $\mu_X(X_{M_{\gamma-\varepsilon-\text{eq}}}) \geq \mu_X(X_M) + \delta$.¹⁰

It is a consequence of these definitions of equilibrium that a system is not always in equilibrium and that it can fluctuate away from equilibrium. This is a radical departure from thermodynamics. It is therefore worth pointing out that this is not merely a concession to the demands of measure-preserving dynamical systems. Having no fluctuations at all is also physically undesirable. There are experimental results that show that equilibrium is not the immutable state that classical thermodynamics presents us with because systems exhibit fluctuations away from equilibrium (MacDonald, 1962; Wang et al., 2002). Hence adopting a notion of equilibrium that allows for fluctuations increases the empirical adequacy of the theory.

⁹ We assume that ε is small enough so that $\alpha(1 - \varepsilon) > \frac{1}{2}$.

¹⁰ We assume that $\varepsilon < \gamma$.

11.3 Local Quantities and Field Variables

The examples we gave in the previous section for relevant macro-variables were internal energy and total magnetisation. These are *global variables*. They assign one value to the entire system, rather than a value to each point in space. Global variables contrast with *local variables*, which are variables like pressure, temperature, and local magnetisation density. These variables assign a value to each point in space. Mathematically speaking, global variables are real valued functions in that they assign a real number to every micro-state in X , and that number is the value of the variable for the micro-state. By contrast, local variables assign a value to each point in space, and if the system is not in equilibrium the values at each point in space will typically vary across the system. For this reason these variables have to be treated as *fields*. We have seen an example of this in Sect. 11.1 when we discussed the pressure of a gas shortly after the removal of the partition wall. In this situation there is no such thing as ‘the’ pressure of the gas and the physical situation is described by a pressure field. In this section we spell out what this means and how fields fit into the framework of LBSM.

Let ordinary physical space be represented by \mathbb{R}^3 . A *scalar field* on \mathbb{R}^3 is a measurable function $f : \mathbb{R}^3 \rightarrow \mathbb{R}$, $\vec{r} \mapsto f(\vec{r})$; i.e. it is a measurable function that assigns each point in space \vec{r} a real number $f(\vec{r})$. Trivially, this definition can be restricted to a subset $S \subseteq \mathbb{R}^3$ and we can say that a scalar field on S is a measurable function $f : S \rightarrow \mathbb{R}$. From a formal point of view, saying that quantities like pressure are ‘local’ means that they are scalar fields. Indeed, pressure and temperature are standard examples of scalar fields. If one wants to restrict the definition of the variable to a particular physical system—for instance to the inside of the container in which the gas is located—then one can say that the variable is scalar field on S , where S is chosen to be the spatial extension of the system.

Let us now consider the set of all scalar fields on \mathbb{R}^3 (or S). It is obvious that this set has the structure of a vector space because the linear combination of any two scalar fields is again a scalar field (assuming the standard definition of the multiplication of function with a number and the addition of two functions). Let us denote this space by \mathcal{F} . The space could be restricted in all kind of ways, for instance by only allowing continuous or differentiable fields. Whether such restrictions are desirable, or even necessary, depends on the physical situation at hand. At the general level no further restrictions are needed. The space can also be endowed with further structures such as norms, inner products and metrics. Again, whether it is advisable, or even necessary, to introduce such additional structures will depend on the physical quantity and the problem at hand; nothing in what we say about scalar fields at the general level depends on having such additional structures in place.

\mathcal{F} contains all scalar fields on \mathbb{R}^3 (or S); that is, all measurable functions $f : \mathbb{R}^3 \rightarrow \mathbb{R}$ (or $f : S \rightarrow \mathbb{R}$). For example, it contains $f(\vec{r}) = 3$, the function that assigns to every point in space the value 3. It also contains $f(\vec{r}) = |\vec{r}|$, the function that assigns to every point in space the value of its distance from the origin. A particular assignment of values to each point of space is also called a *field*

configuration. For example, $f(\vec{r}) = 3$ and $f(\vec{r}) = |\vec{r}|$ are field configurations. So we can say that \mathcal{F} is the space of field configurations.

To see how all this bears on macro-variables in LBSM, recall our observation in the previous section that there is no assumption that *all* \mathbb{V}_i in the definition of a macro-variable have to be \mathbb{R} and that \mathbb{V}_i can in fact be any space. So we are free to take \mathbb{V}_i to be the space \mathcal{F} , and doing so is the key to understanding local variables in LBSM. Indeed, local variables are macro-variables for which \mathbb{V}_i is a space of scalar fields; that is, they are macro-variables that assign to every point in the system's state space a scalar field. For this reason the 'values' of local variable v_i is a field configuration. From a mathematical point of view, we can say that local variables are field-valued variables. Hence, we can say that global variables have the mathematical form of real-valued variables and local variables have the mathematical form of field-valued variables.

It is one of the core posits of LBSM that macro-states are defined by the values of a set of macro-variables $\{v_1, \dots, v_l\}$. Using capital letters V_i to denote the values of v_i , we said that a macro-state was defined by a particular set of values $\{V_1, \dots, V_l\}$: the system is in macro-state M_{V_1, \dots, V_l} iff $v_1 = V_1, \dots, v_l = V_l$. This definition remains valid also after the introduction of fields, but we now have to bear in mind that if a macro-variable is a local variable, then its value is field configuration. One can make this explicit as follows. Assume that for some $k < l$ all v_1, \dots, v_k are real-valued macro-variables and all v_{k+1}, \dots, v_l are field-valued variables. A macro state is then defined though the set of values $\{R_1, \dots, R_k, F_{k+1}, \dots, F_l\}$, where we write ' R ' for real numbers and ' F ' for field configurations. This allows us to define the macro-state of the gas we considered in the Introduction through the triple $\{R_V, F_T, F_p\}$, where R_V is the value of the volume of the gas, F_T is temperature field configuration and F_p is pressure field configuration.

LBSM individuates macro-states through values of macro-variables: two macro-states are identical iff all variables assume the same values. This approach presupposes the notion sameness of values. If the values are real numbers, the notion is trivial: the values are the same if the two real numbers are identical. If the values are functions in a function space, macro-states are individuated by equivalent functions. So in the case of local variables we say two values are the same iff the two functions are equivalent. Different choices to spell out 'equivalent functions' are possible and what notion is adopted will depend on the context. The strictest requirement is to say that two functions f and g from \mathbb{R}^3 or S to \mathbb{R} are equivalent just in case $f(x) = g(x)$ for all x . In measure-theoretic settings it is also natural to say that f and g are equivalent iff they agree for all x except, perhaps, on a set of measure zero.

The introduction of field-valued variables does not change the fact that macro-states supervene on micro-states. The only thing that has changed is that macro-states are now individuated by field configurations rather than values. So it still is the case that micro-states uniquely determine macro-states and that this determination relation is normally many-to-one. It therefore also still is the case that every macro-state M , now defined in terms of field variables, is associated with a *macro-region* X_M consisting of all micro-states for which the system is in M and that for a complete set of macro-states these macro-regions form a partition of X . For this

reasons all other elements of LBSM, in particular the definition of equilibrium, remain unchanged.

As we have previously seen, in some cases it is advisable to define macro-states though intervals rather than exact values. This is straightforward when the values are real numbers, which can easily be ordered in intervals. There is a question how this is best done in the case of field-valued variables. Such a coarse graining could rely, for instance, on a metric on \mathcal{F} and all field configurations that are less than a certain distance away from certain reference field configurations could be seen as belonging to the same macro state. The concrete construction of such a coarse graining depends on the particulars of the situation and there is little one can say at the general level. The point to note here is merely that such coarse grainings can be constructed for field-valued variables just as well as for real-valued variables.

11.4 Physical Realisations

How can relevant physical variables like pressure be defined based on the general formal framework we have outlined in the previous section? A standard way to define local quantities appeals to the so-called Local Equilibrium hypothesis (LEH). In the words of Jou, Vázquez and Lebon the core of LEH is the assumption ‘that the system under study can be mentally split into a series of cells sufficiently large to allow them to be treated as macroscopic thermodynamic subsystems, but sufficiently small that equilibrium is very close to being realized in each cell’ (2010, 14).¹¹ As Öttinger (2005, 39), points out, this can be done, for instance, by imagining the system split up into cubes with a side length of 1mm: such cubes contain a large number of molecules (for air at room temperature the number of particles is of the order of 10^{16}), while at the same time being large with respect to the average mean free path of molecules (which is of the order of 10^{-6} m). Such cubes are at once small enough for relevant quantities to be approximately constant and large enough for thermodynamic concepts to apply. The core of LEH then is that the cubes are systems in thermodynamic equilibrium and that therefore thermodynamic concepts can meaningfully be applied to the cubes. Specifically, quantities like temperature, pressure, entropy are rigorously and unambiguously defined in each cube. The values of these quantities remain constant within a single cube while they can vary across different cubes.

This allows us to define a field: the value of $f(\vec{r})$ is the value that the quantity represented by f assumes in the cube in which \vec{r} lies if the system is in micro-state x . This definition covers the relevant cases. Pressure is defined as force per unit area on the surface of the container when the system is in equilibrium, which implies that it assumes the same value all over the surface. This definition does not, as we

¹¹ For statements and discussions of LEH see Giberti et al. (2019), Jou et al. (2010, 14–15), Spohn (1991, 14), and Öttinger (2005, Ch. 2).

have seen, apply to the entire container as a whole while the gas is spreading; but it applies to a small cube which, by LEH, is in equilibrium. So we can define the pressure in a cube in the same way in which we have previously defined the pressure in the entire vessel. The pressure at point \vec{r} then is simply the pressure in the cube in which the point lies. This unambiguously defines the pressure field across the system.

This definition of the relevant field quantities has the consequence that the field configurations will typically change discontinuously at the boundary between cubes, due to the way in which the cubes are used to define macro-values. This is a drawback because such discontinuous changes are unphysical. This problem can be avoided by changing the definition of local quantities slightly. Rather than first slicing up the system into cubes and then defining the relevant quantities in each cube, one can think of a small cube being placed around each point \vec{r} so that \vec{r} is at the centre of the cube.¹² The size of the cube will be the same as above. This allows us to apply LEH to the cube and say that the cube is in equilibrium, which allows us to define quantities like pressure in the cube. The pressure \vec{r} then is the pressure in the cube around \vec{r} . This way of introducing local quantities has the advantage that it does not introduce discontinuities in the resulting fields through its use of LEH.

The same moves can be made for other variables. Consider the example of temperature. In the context of statistical mechanics temperature T is usually assumed to be proportional to the mean kinetic energy of the system's molecules: $T = 2/3k \langle E_{kin} \rangle$, where $\langle E_{kin} \rangle$ is the particles' mean kinetic energy and k is a constant. We can now make the same moves as with pressure and define the temperature field. The case of densities like the local magnetisation density is even easier. One simply takes the total magnetisation in a cube and divides it by the volume of the cube. In this way fields for all local quantities can be defined.

11.5 Conclusion

In this paper we have shown how local variables such as the pressure of a gas fit into the framework of LBSM. This is a crucial step forward because a unified treatment of equilibrium and non-equilibrium situations can be given only if such variables are available.

Before drawing the discussion to a close we would like to comment on the relation between the well-known thermodynamic distinction between intensive and extensive variables and our distinction between local and global variables. A variable is *extensive* iff it is additive for subsystems. Assume we have two systems S_1 and S_2 and consider a variable v . The values of the variable in the two systems are V_1 and V_2 , respectively. Now we merge the two systems to form a new system S .

¹² Nothing depends on this being a cube. The same construction can be made with a sphere.

The variable v is additive iff the value of v in S is $V_1 + V_2$ (Callen, 1985, 10). Assume now that v has the same value in both systems $V_1 = V_2$. If the value of v in S is also V_1 , then the variable is intensive (*ibid.*, 38). The most obvious example of an extensive variable is volume, because combining two systems will result in a new system whose volume is the sum of the volume of the systems we started with. Other important examples of extensive variables are internal energy and entropy. Examples of intensive variables are temperature and pressure: combining two systems with pressure p and temperature T will result in a larger system which has again pressure p and temperature T .

The point to note is that the two distinctions do not coincide. There is a certain association between them in that important examples of extensive variables are also global (for instance, volume and internal energy) and important examples of intensive variables are also local (for instance, temperature and pressure). But the association is not perfect. The average magnetisation per site in a lattice system is intensive but not local; and the field that assigns to each point the pressure multiplied by the number of molecules in the system is extensive but not global. So the intensive/extensive and local/global distinctions are logically independent.

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