

Phase Transitions: A Challenge for Reductionism?

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Abstract

In this paper, I analyze the extent to which classical phase transitions, especially continuous phase transitions, impose a challenge for reductionism. My main contention is that classical phase transitions are compatible with reduction, at least with the notion of limiting reduction, which relates the behavior of physical quantities in different theories under certain limiting conditions. I argue that this conclusion follows even after recognizing the existence of two infinite limits involved in the treatment of continuous phase transitions.

1 Introduction

Phase transitions are sudden changes in the phenomenological properties of a system. Some common examples include the transition from liquid to gas, from a normal conductor to a superconductor, or from a paramagnet to a ferromagnet. Nowadays phase transitions are considered one of the most interesting and controversial cases in the analysis of inter-theory relations. This is because they make particularly salient the constitutive role played by idealizations in the inference of macroscopic behavior from a theory that describes microscopic interactions. In fact, it appears that statistical mechanics – a well-established microscopic theory – cannot account for the behavior of phase transitions as described by thermodynamics – a macroscopic theory – without the help of infinite idealizations in the form of mathematical limits.

In the discussion on phase transitions, physicists and philosophers alike have mainly been concerned with the use of the thermodynamic limit, an idealization that consists of letting the number of particles as well as the volume of the system go to infinity. For many authors (e.g. Bangu 2009, Bangu 2011; Batterman 2005; Batterman 2011, Morrison 2012) this idealization has an important philosophical consequence: it implies that phase transitions are *emergent phenomena*. As a result, they claim that such phenomena present a challenge for reductionism, i.e. the belief that ultimately all macroscopic laws are reducible to the fundamental microscopic laws of physics.

On the other hand, numerous other authors (e.g. Butterfield 2011; Butterfield and Buoatta 2011; Norton 2012; Callender 2001; Menon and Callender 2013) have rejected this conclusion, arguing that the appeal to the infinite limit does not represent a problem for reductionism. Some of them (Butterfield 2011, Norton 2012) have even argued that phase transitions, instead of threatening reductionism, are paradigmatic examples of Nagelian reduction, whereby reduction is understood in terms of logical deduction.

These last remarks, however, have not ended the debate. In particular, the physical treatment of continuous phase transitions that implements renormalization group (RG) techniques is still regarded as especially problematic for the reductionist attitude towards phase transitions (e.g. Batterman 2011, Morrison 2012).

In this paper, I analyze the extent to which classical phase transitions, especially continuous phase transitions, impose a challenge for reductionism. My main contention is that classical phase transitions are, in fact, compatible with reduction, at least with the notion of reduction that relates the behavior of physical quantities in different theories under certain limiting conditions. I argue that this conclusion follows even if one recognizes the existence of two infinite limits involved in the physics of continuous phase transitions.

To reach my goal, I organize this paper as follows. In the next section (Section 2), I describe the physics of phase transitions, outlining how statistical mechanics recovers thermodynamical behavior. Here I emphasize that in the RG treatment of continuous phase transitions, apart from the thermodynamic limit, there is a second infinite limit involved. Subsequently (Section 3), I further develop the concept of limiting reduction suggested by Nickles (1973). Based on that notion of reduction, I contend (Section 4) that, despite some objections, first-order phase transitions satisfy Nickles' criterion of limiting reduction. However, I also show that continuous phase transitions do not satisfy this criterion due to the existence of the second infinite limit. In Section 5, I suggest to liberalize the notion of limiting reduction and I argue that continuous phase transitions fulfill this notion. This paper concludes by describing some attempts to apply RG methods to finite systems, which indeed support the claim that thermodynamical phase transitions are reducible to statistical mechanics.

2 From Statistical Mechanics to the Thermodynamics of Phase Transitions

Statistical mechanics aims to account for the macroscopic behavior typically described by thermodynamics in terms of the laws that govern microscopic interactions. In the philosophical literature, the reproduction of the thermodynamic results by statistical mechanics is generally referred to in terms of *reduction*. In this section, I will describe how statistical mechanics recovers the thermodynamic behavior of phase transitions and will explain why phase transitions are

an interesting and puzzling case for the project of reducing thermodynamics to statistical mechanics.

2.1 The Thermodynamics of Phase Transitions

In thermodynamics, phases correspond to regions of the parameter space (known as a phase diagram) where the values of the parameters uniquely specify equilibrium states. Phase boundaries, in contrast, correspond to values of parameters at which two different equilibrium states can coexist. The coexistence of states expresses itself as discontinuities of thermodynamic quantities, like volume, which are related to the first derivatives of the free energy with respect to a parameter such as pressure or temperature. If the system goes from one phase to another intersecting a phase boundary, the system is said to undergo a *first-order phase transition*. This name is due to the fact that the discontinuous jumps occur in the first derivatives of the free energy. On the other hand, if the system moves from one phase to another without intersecting any coexistence line, the system is said to undergo a *continuous phase transition*, in which case there are no discontinuities involved in the first derivatives of the free energy but there are divergencies in the response functions (e.g. specific heat, susceptibility for a magnet, compressibility for a fluid). An example of a first-order phase transition is the passage from liquid water to vapor at the boiling point, where the quantities that experience discontinuous jumps are entropy and volume, which are first derivatives of the free energy with respect to temperature and pressure respectively. An example of continuous phase transition instead is the transition in magnetic materials from the phase with spontaneous magnetization – the ferromagnetic phase – to the phase where the spontaneous magnetization vanishes – the paramagnetic phase –. (Figure 1)

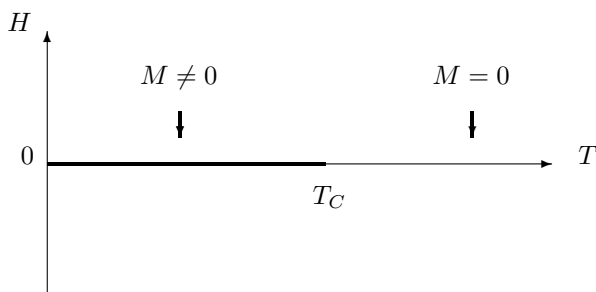


Figure 1: Phase diagram for the paramagnetic–ferromagnetic transition. Here H is the external magnetic field and T the temperature. At the transition or critical point T_C the spontaneous magnetization M vanishes.

Although both first-order and continuous phase transitions are of great interest for the project of reducing thermodynamics to statistical mechanics, the latter kind is considered to be more controversial than the former. The reason is that continuous phase transitions have characteristic properties that are much more difficult to recover from statistical mechanics than first-order phase transitions. One of those properties is that, in the vicinity of a continuous phase transition, measurable quantities depend upon one another in a power-law fashion. For example, in the ferromagnetic-paramagnetic transition, the net magnetization M , the magnetic susceptibility χ , and the specific heat C depend on the reduced temperature $t = \frac{T-T_c}{T_c}$ (the temperature of the system with respect to the critical temperature T_c) as follows:

$$M \sim |t|^\beta, C \sim |t|^{-\alpha}, \chi \sim |t|^{-\gamma},$$

where β , α , γ are the *critical exponents*. Another remarkable property of continuous phase transitions is that radically different systems, such as fluids and ferromagnets, have exactly the same values of critical exponents, a property known as *universality*.

Finally, continuous phase transitions are also characterized by the divergence of some physical quantities at the transition or critical point. The critical exponents α and γ are typically (although not always) positive, so that the power laws that have negative exponents (and the corresponding quantities like specific heat and susceptibility) diverge as $T \rightarrow T_c$. The divergence of the magnetic susceptibility χ implies the divergence of the *correlation length* ξ , a quantity that measures the distance over which the spins are correlated, which also obeys power-law behavior: $\xi \sim |t|^{-\nu}$. The divergence of the correlation length is perhaps the most important feature of continuous phase transitions because it involves the loss of a characteristic scale at the transition point and thus provides a basis for universal behavior.

The inference of the experimental values of critical exponents – or adequate relations among them – together with the account of universality has been one the major challenges of statistical mechanics. We will see next that, in order to provide such an account, it was necessary to appeal to infinite idealizations and to RG methods, an entirely new theoretical framework, which basically consists in reducing the number of effective degrees of freedom of the system.

2.2 The Importance of the Thermodynamic Limit

We saw in the previous section that the macroscopic behavior of first-order phase transitions is defined in terms of singularities or non-analyticities in the first derivatives of the free energy. Gibbsian statistical mechanics offers a precise definition of the free energy F , given by:

$$F(K_n) = -\kappa_B T \ln Z, \tag{1}$$

where K_n is the set of coupling constants, κ_B is the Boltzmannian constant, T is the temperature, and Z is the canonical partition function, defined as the

sum over all possible configurations:

$$Z = \sum_i e^{\beta H_i}. \quad (2)$$

When trying to use statistical mechanics to recover the non-analyticities that describe phase transitions in thermodynamics, the following problem arises. Since the Hamiltonian H is usually a non-singular function of the degrees of freedom, it follows that the partition function, which depends on the Hamiltonian, is a sum of analytic functions. This means that neither the free energy, defined as the logarithm of the partition function, nor its derivatives can have the singularities that characterize first-order phase transitions in thermodynamics. Taking the thermodynamic limit, which consists of letting the number of particles as well as the volume of the system go to infinity $N \rightarrow \infty$, $V \rightarrow \infty$ in such a way that the density remains finite, allows one to recover those singularities. In this sense, the use of this limit appears essential for the recovery of the thermodynamic values, which motivated Kadanoff’s controversial claim: “phase transitions cannot occur in finite systems, phase transitions are solely a property of infinite systems” (Kadanoff, 2009, p. 7).

The appeal to the thermodynamic limit is also found in the description of continuous phase transitions. Consider again the paramagnetic-ferromagnetic transition. This is a continuous phase transition defined in terms of the divergence of the magnetic susceptibility at the critical temperature and characterized by the appearance of spontaneous magnetization in the absence of an external magnetic field. From a statistical mechanical point of view, the appearance of spontaneous magnetization in finite systems is, strictly speaking, impossible. The impossibility is due to the up-down symmetry of the lattice models used in the study of magnetization, including the Ising model. A consequence of up-down symmetry is that for zero external field H the magnetization obeys the symmetry condition $M = -M$, whose unique solution is $M = 0$. That means that the magnetization M with zero external magnetic field H must be zero (Details elsewhere, e.g. Goldenfeld 1992, Sec. 4; Le Bellac, Mortessagne, and Batrouni 2006, Sec. 4). This so-called “impossibility theorem” can be avoided by taking the thermodynamic limit $N \rightarrow \infty$ followed by the limits $H \rightarrow 0^+$ and $H \rightarrow 0^-$:

$$M = \lim_{H \rightarrow 0^+} \lim_{N \rightarrow \infty} \frac{1}{N} \frac{\partial F(H)}{\partial H} \neq 0$$

$$-M = \lim_{H \rightarrow 0^-} \lim_{N \rightarrow \infty} \frac{1}{N} \frac{\partial F(H)}{\partial H} \neq 0.$$

Notice that since M and $-M$ have different values and are different from zero, the magnetic susceptibility, defined as the derivative of the magnetization with respect to an external field, diverges to infinity in the neighborhood of the zero external field. One can see, therefore, that taking the thermodynamic limit not only provides the concept of spontaneous magnetization with precise

meaning but also allows for the recovery of the divergence of the thermodynamic quantities that characterizes continuous phase transitions.

2.3 The Appeal to a Second Limit: Infinite Iteration of RG Transformations

In an ideal scenario, one would expect to perform a direct calculation of the partition function. Unfortunately, analytic calculations of the partition functions have been performed only in particular models with dimension $D = 1$ or $D = 2$; for all other cases, one requires to use approximation techniques.¹ The most useful approximation for the case of first-order phase transitions is the *mean field approximation*, which employs the assumption that each spin acts as if it were independent of the others, feeling only the *average mean field*. Although the mean field approximation proved to be successful in some cases of first order phase transitions, experiments have shown that this account fails to give accurate predictions for the case of continuous phase transitions, in which the correlation length diverges. It is believed that this failure is due to the fact that mean field theories neglect fluctuations whereas fluctuations govern the behavior near the critical point.

A more complete account of continuous phase transitions requires the use of RG methods. These methods are mathematical and conceptual tools that allow one to solve a problem involving long-range correlations by generating a succession of simpler (generally local) models. The goal of these methods is to find a transformation that successively coarse-grains the effective degrees of freedom but keeps the partition function and the free energy (approximately) invariant. The usefulness of RG methods lies in the fact that one can compute the critical exponents and other universal properties without having to calculate the free energy. This methods also allow to account for universality, the remarkable fact that entirely different systems behave qualitatively and quantitatively in the same way near the critical point.

To give a specific illustration of RG methods, let us consider a block spin transformation for a simple Ising model on the two-dimensional square lattice with distance a between spins.² Here, the spins have two possible values, namely ± 1 . If it is assumed that the spins interact only with an external magnetic field h and with their nearest neighbors through the exchange interaction K (meaning that the coupling constants are only K and h), the Hamiltonian H for the model is given by:

$$H = -K \sum_{ij}^N S_i S_j + -h \sum_i S_i. \quad (3)$$

¹The first and most famous exact solution of the partition function is the Onsager solution for an Ising model of dimension $D=2$.

²For simplicity, I am going to restrict the analysis to real-space renormalization. However, I think that the same conclusions apply to momentum-space renormalization. For details on the difference between real-space and momentum space-renormalization, see Wilson and Kogut (1974) and Fisher (1998). For a philosophical account on the difference between those two frameworks see Franklin (2017)

By applying the majority rule, which imposes the selection of one state of spin based on the states of the majority of spins within a block, one can replace the spins within a block of side la by a single *block spin*. Thus, one obtains a system that provides a coarse-grained description of the original system.

If one assumes further that the possible values for each block spin S_I are the same as in the Ising model, namely ± 1 , and also that the block spins interact only with nearest neighbor block spins and an external field, the effective Hamiltonian H' will have the same form as the original Hamiltonian H :

$$H' = -K' \sum_{IJ}^{Nl^{-d}} S_I S_J + -h' \sum_I S_I. \quad (4)$$

Formally, this is equivalent to applying a transformation R to the original system, so that $H' = R[H]$, in which the partition function and the free energy remain approximately invariant.³

Although the systems described by H and H' have the same form, the correlation length in the coarse-grained system $\xi[K']$ is smaller than the correlation length $\xi[K]$ of the original system. This follows from the fact that the correlation length in the effective model is measured in units of the spacing la whereas the correlation length in the original system is measured in units of the spacing a . In other words, the correlation length is rescaled by a factor l . The expression that relates the correlation lengths of the two systems is:

$$\frac{\xi[K]}{l} = \xi[K']. \quad (5)$$

After n iterations of the RG transformation, the characteristic linear dimension of the system is l^n . Thus the correlation lengths in the sequence of coarse-grained models vary according to:

$$\xi[K] = l\xi[K'] = \dots = l^n \xi[K^{(n)}]. \quad (6)$$

The idea is that one iterates the RG transformation until fluctuations at all scales up to the physical correlation length ξ are averaged out. In many cases, this involves numerous iterations (Details elsewhere, e.g. Le Bellac et al. 2006, Sec. 4.4.3; Goldenfeld 1992, Sec. 9.3).

It follows from equation (6) that for a large correlation length, the number of iterations should be large. For an infinite correlation length, which is the case of continuous phase transitions, the number of iterations should be infinite.⁴ Indeed, if the original correlation length $\xi[K]$ is infinite and we want to eliminate all effective degrees of freedom, i.e. we want the effective correlation length to

³The previous example captures the spirit of real-space RG methods. However in practice RG transformations consist of complicated non-linear transformations that do not preserve the form of the original Hamiltonian. This allows for the possibility that new local operators are generated during the RG transformation (Details in Goldenfeld 1992, p. 235).

⁴In order to maintain the system at criticality, one performs a sort of double rescaling process: one changes scale in space and also changes the distance to criticality in coupling space (Details in Sornette 2000, p. 232).

be small, then we are forced to take the limit $n \rightarrow \infty$ in the right hand side of equation (6) such that the following expression holds:

$$\xi[K] = \lim_{n \rightarrow \infty} l^n \xi[K^{(n)}] = \infty \quad (7)$$

This result is important because it demonstrates the existence of two different infinite limits involved in the theory of phase transitions. The first is the thermodynamic limit that takes us to a system with an infinite correlation length. The second is the limit for the number of RG iterations going to infinity that takes us to a fixed point Hamiltonian, i.e. the Hamiltonian with the coupling constants equal to their fixed point values: $[K^*] = R[K^*]$. These fixed points can be also thought of as stationary or limiting distributions to which the renormalization group trajectories converge after infinite iterations of the RG transformation $n \rightarrow \infty$. This point will be crucial for what will be argued in Sections 3.3 and 5.2.

Although the iteration of the RG transformation preserves the symmetries of the original system, it does not preserve the value of the original Hamiltonian, and, therefore, it does not preserve the value of the set of coupling constants $[K]$ associated with the corresponding Hamiltonians. Thus, the iteration of the RG transformation can be thought of as describing a sequence of points moving in a space of coupling constants K^n or a corresponding space of Hamiltonians H . If the sequence describes a system at the critical point, after infinite iterations $n \rightarrow \infty$ it will converge to a non-trivial fixed point $[K^*]$ given by:

$$[K^*] = R[K^*] \quad (8)$$

The other possible fixed points are trivial, namely $K = 0$ and $K = \infty$, which correspond to low and high temperature fixed points respectively.

At fixed points the coupling constants remain invariant under the transformation. Therefore, varying the length scale does not change the value of the Hamiltonian and therefore brings us to a physically identical system. This latter feature associates fixed points with the property of scale invariance, which means that the system looks statistically (and physically) the same at different scales.

It has been shown that by linearizing in the vicinity of the fixed point, one can calculate the values of the critical exponents and the relations between them (Details in Goldenfeld 1992, Sec. 9; Domb 2000, Sec. 7; Sornette 2000, Sec. 11). This is remarkable because it demonstrates that the critical exponents are solely controlled by the RG trajectory near the fixed point and that one does not need to calculate the free energy to determine the behavior of the system in the vicinity of the critical point. This means also that the initial values of the coupling constants do not determine the critical behavior. The latter constitutes the origin of the explanation of *universality* because it tells us that systems that flow towards the same fixed point are governed by the same critical exponents, even if they are originally described by different coupling constants. The systems that flow towards the same fixed point – that are in the basin of attraction of the fixed point – are said to be in the same *universality class*.

In summary, we have seen that the recovery of the thermodynamic properties from statistical mechanics involves: i) first, the introduction of particular assumptions (e.g. lattice structure, a particular kind of degrees of freedom, ranges of values of the degrees of freedom, and dimension) that allow one to build a specific model (Ising model in our case study); ii) second, the assumption of the thermodynamic limit, which brings us to a fine-grained system with infinite number of particles and infinite correlation length;⁵ and iii) finally, the assumption of a second infinite limit that consists of an infinite number of iterations of a coarse-graining transformation. This limit takes us to a fixed point Hamiltonian that represents a coarse-grained model. After those steps are made, the most important statistical mechanical approaches can make accurate predictions of the behavior of continuous phase transitions and explain universal behavior. Figure 2 illustrates this process. Notice, however, that in the case of first-order phase transitions, one could in principle derive the thermodynamic behavior just after taking the first limit.⁶

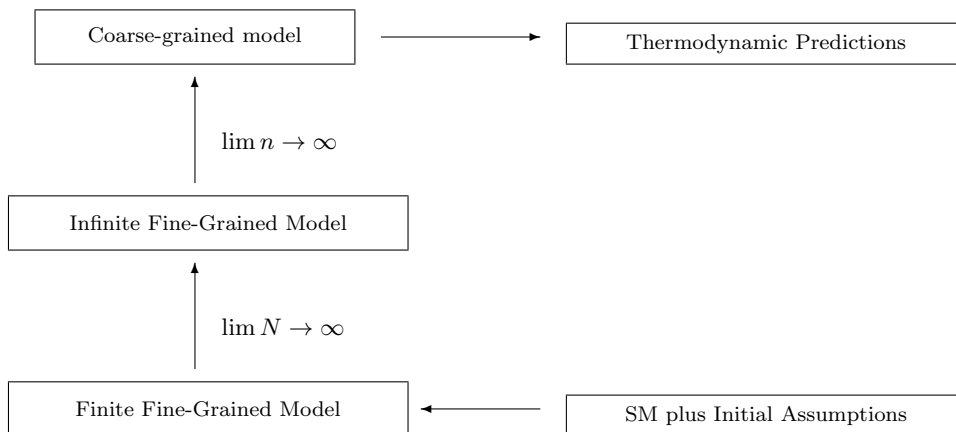


Figure 2: Inter-theory relation for continuous phase transitions.

⁵Recently, Norton (2012) has challenged the appeal to an infinite system in the theory of phase transitions. His contention is that the limit system would have properties that are not suitable to describe phase transitions, such as the violation of determinism and energy conservation. This point is relevant for his distinction between idealizations and approximations, which led him to the conclusion that phase transitions are a case of approximation and not idealization. Since we are trying to make a different point here, we are going to adhere to the standard *façon de parler* that refers to the existence of an “infinite system” (e.g. Kadanoff 2009; Fisher 1998; Butterfield 2011). This does not mean that our view is incompatible with Norton’s view.

⁶One should bear in mind that although RG methods are not required to infer the behavior of first-order phase transitions, they can be (and have been) used to describe these kinds of transitions as well. See Goldenfeld (1992, Sec. 9).

3 The Concept of Limiting Reduction

What has been at stake in the philosophical debate around phase transitions is whether the thermodynamic description of these phenomena *reduces* to statistical mechanics. Even if the previous section showed that statistical mechanics can reproduce the non-analyticities that describe phase transitions in thermodynamics, the appeal to the infinite idealizations throws suspicion to the legitimacy of such a reduction. The main aim of Sections 4 and 5 is to evaluate whether the infinite idealizations mentioned in Section 2 are compatible with the reduction of phase transitions. However, given that the term “reduction” is notoriously ambiguous, before we can assess this issue, some clarifications as to how this term is constructed in this context are necessary. This is the task of the present section.

3.1 Nickles’ Concept of Limiting Reduction

Since we are interested in relating the thermodynamic treatment of phase transitions with another theory that aims to describe the same phenomena, we are treating phase transitions as a potential case of inter-theory reduction, where reduction is taken as a relation between two theories (or parts of theories). This kind of reduction is to be distinguished from other types of reduction such as whole-parts reduction.⁷ More specifically, since the description of the phenomenon in the two theories coincides only by assuming a limit process, the case of interest is a candidate for a specific class of inter-theory reduction sometimes called *limiting* or *asymptotic* reduction (Landsman, 2013).

Nickles (1973, pp. 197-201), who was the first to distinguish *limiting* reduction from other classes of inter-theory reduction, calls this type of reduction *reduction₂* (henceforth LR_2) to distinguish it from *reduction₁*, which corresponds to Nagelian reduction. He characterizes LR_2 in the following way:

LR_2 : A theory T_B (secondary theory) reduces to another T_A (fundamental theory), iff the values of the relevant quantities of T_A *become* the values of the corresponding quantities of T_B by performing a limit operation on T_A .⁸

According to Nickles, the motivation for this type of reduction is heuristic and justificatory. The development of the new (or fundamental) theory T_A is motivated heuristically by the requirement that, in the limit, one obtains the same values as the predecessor (or secondary) theory T_B for the relevant quantities. As such, T_A is also justified as it can account adequately for the domain

⁷See Norton (2012) for a clear distinction between these two kinds of reduction.

⁸Nickles (1973) inverts the order of “reducing” theory and theory “to be reduced” used by philosophers. According to him, the “reducing theory” is the theory that results from the limit operation and the theory “to be reduced” is the theory in which the limit operation is performed. This terminology is motivated by the way in which physicists use the term “reduce to”. Since this notation is not relevant for Nickles’ general concept of limiting reduction, I will use the term according to the philosophers’ jargon and not following Nickles’ terminology.

described by T_B . Nickles is also emphatic in pointing out that this kind of reduction is to be distinguished from *reduction*₁, which, as I said above, corresponds to Nagelian reduction. He clarifies that whereas Nagelian reduction requires the old (or secondary) theory to be embedded entirely in the new theory, limiting reduction only requires that the two theories make the same predictions for the relevant quantities when a limiting operation is performed. In this way, *reduction*₂, in contrast to *reduction*₁, does not require the logical derivation of one theory from another and, therefore, does not require logical consistency between the two theories (Nickles, 1973, p. 186). Since Nickles' *reduction*₂ does not make any reference to explanation, logical deduction or the ontological status of reduction, which are aspects of more standard philosophical conceptions of reduction, this type of reduction is often regarded as the “physical sense” of reduction (e.g. Nickles 1973; Rohrlich 1988; Batterman 2016).

3.2 Beyond Nickles' Concept of Reduction

In order to evaluate potential cases of limiting reduction, it is useful to have a formal definition at hand. Batterman (2016) advances such a definition by proposing the following schema (which he calls *Schema R*, henceforth *SR*):

SR: A theory T_B reduces asymptotically to another T_A iff:

$$\lim_{x \rightarrow \infty} T_A = T_B,$$

where x represents a fundamental parameter appearing in T_A . T_A is generally taken as the fundamental theory and T_B is typically taken as a secondary or coarser theory.⁹ For Batterman, the relation between two theories can be called “reductive” if the solutions of the relevant laws of the theory T_A smoothly approach the solutions of the corresponding laws in T_B , or in other words, if the “limiting behavior” of the relevant laws, with $x \rightarrow \infty$, *equals* the “behavior in the limit”, where $x = \infty$.

It could be objected, however, that Batterman's *Schema R* is not precise enough since, strictly speaking, the limit is taken on functions representing quantities (or properties) of a theory rather than on the theory itself. Moreover, even if two functions representing the same physical quantity in T_A and T_B respectively coincide when a limit is taken, that does not guarantee the reduction of an entire theory to another. In fact, it might be possible for the functions representing a given quantity in the fundamental and secondary theory to be related by limiting reduction while for another quantity the corresponding functions fail to do so. A more precise definition of limiting reduction, formulated only in terms of the quantities to be compared, is as follows:

⁹In the original formulation, Batterman (2016) defines schema R, using $\epsilon \rightarrow 0$ instead of $x \rightarrow \infty$. For consistency with other parts of this paper, I instead express schema R as considering the limit to infinity $x \rightarrow \infty$. Whether one formulates $x \rightarrow \infty$ or $\epsilon \rightarrow 0$ does not make a difference in the content of this schema.

LR_3 : A quantity Q^B of T_B reduces asymptotically to a quantity Q^A of T_A if:

$$\lim_{x \rightarrow \infty} Q_x^A = Q^B,$$

where x represents a parameter appearing in T_A , on which the function representing Q_x^A depends. According to this definition, one is thus allowed to call a relation between quantities “reductive” if the values of the quantity Q_x^A smoothly approach the values of the quantity Q^B when the limit $x \rightarrow \infty$ is taken. Naturally, in order to obtain the reduction of one theory to another, one would require that the values of *all* the physically significant quantities of the reduced theory coincide with the values of the quantities of the fundamental theory under certain conditions.¹⁰ Proving this in every case is a huge enterprise, but note that, according to the above framework, the failure of reduction of one of the relevant quantities suffices to infer the failure of reduction of an entire theory to another. As it will be seen in the next section, this is exactly what is at stake in the case of phase transitions.

Before going there though, more specifications regarding the concept of limiting reduction are necessary. For example, it can still be argued that definition LR_3 is far too strict since it requires that the values obtained by performing a limit operation on a quantity Q_x^A are exactly the same as the values of Q^B . In most cases this condition is not satisfied. Take, for instance, the concept of entropy as it is defined in thermodynamics and in Boltzmannian statistical mechanics. In thermodynamics, such a quantity reaches its maximum value at equilibrium and does not allow for fluctuations. In contrast, Boltzmannian entropy is a probabilistic quantity that fluctuates every now and then even when the system has reached equilibrium. Cases like this motivated many authors (including Nickles himself) to allow for “approximate reduction”. Accordingly, one can reformulate LR_3 as follows :

LR_4 : A quantity Q^B of T_B reduces asymptotically to a quantity Q^A of T_A if:

$$\lim_{x \rightarrow \infty} Q_x^A \approx Q^B,$$

where “ \approx ” means “approximates”, “is similar to”, or “is analogous to”. This means that a quantity Q_x^A reduces another quantity Q^B if the values of Q_x^A *approximate* the values of Q^B when the limit $x \rightarrow \infty$ is taken.

¹⁰Note, however, that here we assume that the two quantities have some qualitative features in common that make them candidates for reduction. An important topic that deserves to be addressed in future research regards the issue of whether quantitative coincidence suffices to infer correspondence between two quantities of different theories.

4 Are Continuous Phase Transitions Incompatible with Reduction?

In order to judge whether phase transitions correspond to a case of reduction, one needs to specify which quantities of T_A and T_B are expected to display the same values when a certain limit is taken. Subsequently, one needs to evaluate whether these quantities relate to each other according to the definitions provided in the previous section.

In both first-order and continuous phase transitions one is interested in comparing quantities of statistical mechanics with quantities of classical thermodynamics, where statistical mechanics is taken as the reducing theory T_A and classical thermodynamics as the theory to be reduced T_B . As it was shown in Section 2.2, in the case of first-order phase transitions one takes the thermodynamic limit to obtain the singularities in the derivatives of the free energy that successfully describe the phenomenon in thermodynamics. Following definition LR_4 , one will say that the derivatives of the free energy in thermodynamics are reduced to the corresponding quantities in statistical mechanics if

$$\lim_{N \rightarrow \infty} F_N^{SM} \approx F^{TD},$$

where F^{SM} represents a derivative of the free energy as defined in statistical mechanics and F^{TD} the corresponding quantity in thermodynamics.

The case of continuous phase transitions is different, because, in general, one is not interested in computing the free energy but rather in calculating the universal quantities, like the critical exponents, and in explaining universality. In other words, one uses the thermodynamic limit and the infinite iteration limit to calculate the critical exponents that control the behavior of the system close to the critical point.

4.1 The Problem of “Singular” Limits

The view that phase transitions are not a case of limiting reduction has been most notably developed by Batterman (2001; 2005; 2011). He argues that this is a consequence of the “singular” nature of the thermodynamic limit.¹¹

Using Batterman’s terminology, a limit is singular “if the behavior in the limit is of a *fundamentally different character* than the nearby solutions one obtains as $\epsilon \rightarrow 0$ ” (Batterman, 2005, p. 2). According to him, the thermodynamic limit is *singular* in this sense because no matter how large we take the number of particles N to be, as long as the system is finite, the derivatives of the free energy will never display a singularity. As a consequence, he says that taking the limit of the free energy of finite statistical mechanics F^{SM} does not allow us to construct a model or theory that approximates the thermodynamic behavior.

The idea that we can find analytic partition functions that “approximate” singularities is mistaken, because the very notion of approx-

¹¹Similar views are also held by Rueger (2000) and Morrison (2012).

imation required fails to make sense when the limit is singular. The behavior at the limit (the physical discontinuity, the phase transition) is qualitatively different from the limiting behavior as that limit is approached (Batterman, 2005, p. 14).

This means that phase transitions would not even satisfy definition LR_4 stated in Section 4.

Although Batterman’s argument is plausible, Butterfield (2011) (and Butterfield and Buoatta (2011)) challenges his reasoning using the following mathematical example. Consider the following sequence of functions:

$$g_N(x) = \begin{cases} -1 & \text{if } x \leq -1/N \\ N_x & \text{if } -1/N \leq x \leq 1/N \\ 1 & \text{if } x \geq 1/N \end{cases}$$

As N goes to infinity, the sequence converges pointwise to the discontinuous function:

$$g_\infty(x) = \begin{cases} -1 & \text{if } x < 0 \\ 0 & \text{if } x = 0 \\ 1 & \text{if } x > 0 \end{cases}$$

If one introduces another function f , such that

$$f = \begin{cases} 1 & \text{if } g \text{ diverges} \\ 0 & \text{if } g \text{ does not diverge} \end{cases}$$

then one will conclude, in the same vein as Batterman, that the value of f_∞ at the limit $N = \infty$ is *fundamentally different* from the value when N is arbitrarily large but finite. However, Butterfield warns us that if we look at the behavior of the function g , we will see that the limit value of the function is approached smoothly and therefore that the limit system is not “singular” in the previous sense.

According to Butterfield, this is exactly what happens with classical phase transitions and, for the cases analyzed here, he seems right.¹² Consider again the paramagnetic-ferromagnetic transition discussed in Section 2.1. This transition is characterized by the divergence of a second derivative of the free energy - the magnetic susceptibility χ - at the critical point. If we introduce a quantity that represents the divergence of the magnetic susceptibility and attribute a value 1 if the magnetic susceptibility diverges and 0 if it does not (analogously to the function f in Butterfield’s example), then we might conclude that such

¹²Even if Butterfield aims to make a more general claim, this does not hold for all cases of “singular” limits. Landsman (2013) shows that for the case of quantum systems displaying spontaneous symmetry breaking and the classical limit $\hbar \rightarrow 0$ of quantum mechanics, the situation is different and much more challenging. It seems therefore that the analysis of singular limits and the way of “dissolving the mystery” around them should be done on a case-by-case basis.

a quantity will have values for the limit system that are considerably different from the values of the of systems close to the limit, i.e. for large but finite N . As a consequence, we will say that definition LR_4 fails. However, if we focus on the behavior of a different quantity, namely the magnetic susceptibility itself χ , we will arrive at a different conclusion. In fact, as N grows, the change in the magnetization becomes steeper and steeper so that the magnetic susceptibility smoothly approaches a divergence in the limit (analogous to the function g). This result is important because it tells us that definition LR_4 holds:

$$\lim_{N \rightarrow \infty} \chi_N^{SM} \approx \chi^{TD},$$

where χ^{SM} and χ^{TD} are taken as the magnetic susceptibility in statistical mechanics and thermodynamics respectively. The existence of finite statistical systems whose quantities approximate qualitatively the thermodynamic quantities for the case of first-order and continuous phase transitions has been also corroborated by Monte Carlo simulations (I will come back to this point in Section 6).

The important lesson from Butterfield’s argument is that the “singular” nature of the thermodynamic limit does not imply that there are no models of statistical mechanics that approximate the thermodynamic behavior of phase transitions, for N sufficiently large but finite. If we assume that inter-theory reduction is consistent with the fact that the quantities of the secondary theory are only approximated by the quantities of the fundamental theory (as suggested by schema LR_4), then we arrive at the important conclusion that the “singular” nature of the thermodynamic limit is not *per se* in tension with the reduction of phase transitions.

One needs to be cautious, however, in not concluding that the previous argument solves all the controversy around the reduction of phase transitions. First of all, it is important to bear in mind that we are referring only to classical phase transitions and that quantum phase transitions have not been considered.¹³ Second, one needs to note that we have not considered the use of renormalization group methods yet, in which there are two infinite limits involved. This is precisely the issue that we are going to address next.

4.2 Implementing RG Methods

As was shown in Section 2, the inference of the thermodynamic behavior of continuous phase transitions generally requires the appeal to RG methods. Batterman (2011) has suggested that the assumption of RG methods imposes a further challenge for the project of reducing phase transitions to statistical mechanics. He attributes this difficulty to the need for the thermodynamic limit in the inference of fixed point solutions, which are said to be necessary for the computation of critical exponents and for giving an account of universality. He claims (2011, p. 23):

¹³For an analysis of quantum phase transitions see Landsman (2013).

Notice the absolutely essential role played by the divergence of the correlation length in this explanatory story. It is this that opens up the possibility of a fixed point solution to the renormalization group equations. Without that divergence and the corresponding loss of characteristic scale, no calculation of the exponent would be possible.

Why is it that the thermodynamic limit appears to be so important in the inference of non-trivial fixed points? The reason is that in every finite system there will be a characteristic length scale associated to the size of the system. Therefore, the application of a coarse-graining transformation beyond that length will no longer give identical statistical systems and the “RG flow” will inevitably move towards a trivial fixed point, with values of the coupling constants either $K = 0$ or $K = \infty$.

Figure 3 describes a contour map sketching the topology of the renormalization group flow and serves to illustrate the previous situation. Here the RG flows are represented by the trajectories R and D in a space S of Hamiltonians. Each point in this space represents a physical system described by a particular Hamiltonian associated with a set of coupling constants K . In this topology, the elements of S can be classified according to their correlation lengths ξ . Therefore, one can define surfaces containing all Hamiltonians $H \in S$ with a given correlation length. For example, the critical surface describes the set of all Hamiltonians with infinite correlation length $\xi = \infty$. In the figure, p represents a system with a Hamiltonian that inhabits the critical surface $\xi = \infty$, whereas s represents a system with a Hamiltonian that is infinitesimally close to p but is not on the critical surface; p^* and p_0 are fixed points. As one can see, the trajectory starting from s will stay close to trajectory R , describing a system at criticality, but eventually will move away towards a trivial fixed point. This follows because in a finite system the RG transformation will constantly reduce the value of the correlation length, moving the system away from criticality and resulting in a system with trivial values of coupling constants. As a result, two neighbor systems will approach far away fixed-points when a RG transformation is repeated infinitely many times, i.e. when $n \rightarrow \infty$, and therefore the two neighbor systems will approach two different limiting distributions describing physically diverse systems. Since the values of the critical exponents can be calculated by linearizing around non-trivial fixed points, this naturally means that iterating the RG transformation infinitely many times in a finite system will lead us to a fixed point from which one will be able neither to compute the critical exponents nor to give an account of universality. Taking into account that the critical exponents describe the behavior of the physical quantities Q close to the critical point, one can formally express this fact as follows. For N being arbitrarily large but finite:

$$\lim_{n \rightarrow \infty} Q_{N,n}^{SM} \not\approx Q^{TD},$$

where n is the number of iterations, Q^{SM} represents a quantity of statistical

mechanics controlled by the critical exponents, whereas Q^{TD} represents the corresponding quantity in thermodynamics whose values match with the experimental results.

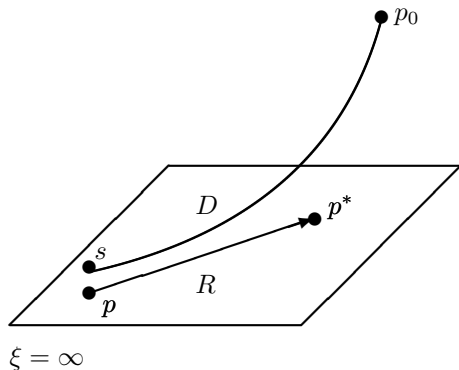


Figure 3: Contour map sketching the topology of the renormalization group flow (R). s and p represent systems infinitesimally close to each other. p^* is a critical fixed point and p_0 is a trivial-fixed point.

This is what led Batterman and others, for example Morrison (2012), to stress the importance of the thermodynamic limit. In fact, one can see from the argument given above that only systems with infinite correlation length (associated with a loss of characteristic scale) will approach non-trivial fixed points after infinite iterations of the RG transformation. The point that these authors do not emphasize is, however, that it is by taking the *infinite iteration limit* $n \rightarrow \infty$ that one approaches trivial fixed points from which one can neither explain universality nor calculate the critical exponents. If one realizes this, then the question that arises is whether in a finite system one can recover the experimental values of the critical exponents only after a finite number of iterations of the renormalization group transformations, i.e. without taking the second limit. This will be addressed in the next section.

5 Approximation, Topology and the Reduction of Continuous Phase Transitions

Before assessing the reducibility of continuous phase transitions, let us discuss the notion of approximation involved in the concept of limiting reduction. In the definition suggested by Nickles (and also in the revised versions mentioned

in Section 4), there is implicit a precise criterion of approximation given by the convergence of the values of quantities in the fundamental theory to the values of the corresponding quantities in the secondary theory (See also Scheibe 1998, Hüttermann and Love 2016, Fletcher 2015).¹⁴ We saw that, in cases where the quantitative and qualitative behavior of phase transitions can be inferred solely by taking the thermodynamic limit, this criterion of approximation well captures the idea of the reducibility of the quantities that describe phase transitions. The cases mentioned in Section 4.1 are examples of this.

Unfortunately, one cannot use the same criterion of approximation in cases in which taking the thermodynamic limit is not sufficient to infer the thermodynamic behavior. The reason is that, as we saw, in the case of continuous phase transitions one generally infers the thermodynamic behavior and explains universality only after performing a second limiting operation, which consists of applying repeatedly an RG transformation in the parameter space until the trajectory converges towards a non-trivial fixed point. Such a convergence does not, however, give us the criterion of approximation that can be used to determine whether phase transitions are a case of reduction. This is because when we ask about reduction, we are interested in analyzing the behavior of finite systems. Instead, the points of the RG trajectory describing a system at criticality are confined to the critical surface, corresponding to points with infinite correlation length $\xi = \infty$, and that does not give us any information about the behavior of finite systems.

The challenge that the reductionist needs to face is that every point in a space of coupling constants that describes a system with finite correlation length will approach a trivial fixed point when the infinite iteration limit is taken. In this sense, if one sticks to the criterion of convergence to establish similarity or approximation between different physical quantities, one will conclude that the values of the quantities of statistical mechanics do not approximate the values of thermodynamic quantities. As a consequence, and in agreement with Batterman (2011), one would claim that limiting reduction fails for the case of continuous phase transitions.

But, what forces us to understand approximation only in terms of convergence towards a certain limit? Imagine that we could delimitate a region in the neighborhood of a fixed point p^* , as illustrated in Figure 4. Imagine further that we could show that the RG trajectory D generated by a finite system s intersects the region U around the fixed point p^* , after a large but finite number of iterations. Finally, imagine that linearizing around a point d' of the trajectory D which resides inside the region U allows us to calculate, at least approximately, the experimental values of the critical exponents. Could we say, then, that we have succeeded in deriving, at least approximately, the experimental values of the physical quantities from finite statistical mechanics? I think we could. Let me now show that this is actually the case.

¹⁴The convergence involved in limiting relations is generally pointwise and not uniform.

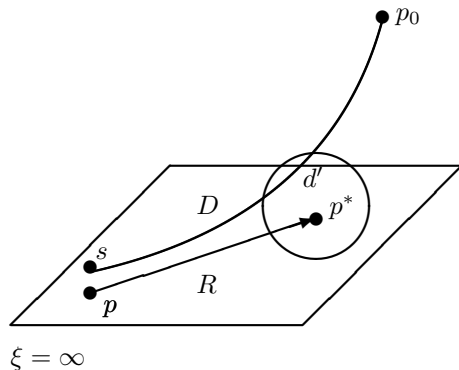


Figure 4: The region around the fixed point p^* represents neighboring points.

Wilson and Kogut (1974, Sec. 12) demonstrated by using ϵ -expansion approximation that in principle, and for an idealized case, if one starts from a point which is close enough to the critical surface, the RG trajectory will move close to the critical trajectory until it reaches the vicinity of a non-trivial fixed point p^* .¹⁵ Once the trajectory reaches the neighborhood U of the fixed point p^* will stay there for a long time (which means, for repeated iterations of the RG transformation), thereby acting as it were a fixed-point. Finally, as $n \rightarrow \infty$, the trajectory will eventually move away from that region approaching a trivial fixed point.

What is relevant for us is that within the neighborhood U of the fixed point linearization is indeed possible, which implies that from a finite system one can obtain the values of the critical exponents after a finite number of iterations of the RG transformation. In order to derive accurate values of the critical exponents, the number of iterations of the RG transformations should be large enough so that all details which are not universal, namely all details specific to a model, are washed out. If the number of iterations is not large enough the coupling constants will be sensitive to details of the model and the calculations of critical exponents will not be accurate (For details see also Le Bellac 1998).

If the ultimate goal of limiting reduction is to justify the fundamental theory by showing that the relevant quantities display values that approximate the values of the secondary theory, then, based on the previous argument, we have good reason to say that the quantities that describe continuous phase transitions in thermodynamics reduce to the quantities that describe the same phenomena in statistical mechanics, at least in this idealized case.

The formal expression that describes reduction in this particular case is as

¹⁵The ϵ -expansion is an asymptotic expansion for which ϵ takes values from $\epsilon = 1$ to $\epsilon \ll 1$. Since the exponents are not analytic at $\epsilon = 0$ one faces convergence problems which are treated by sophisticated summation methods that are nowadays under control.

follows:

LR₅: A physical quantity Q^{SM} in statistical mechanics reduces asymptotically to the analogous quantity Q^{TD} in thermodynamics, if for N sufficiently large:

$$\exists n_0 \text{ such that } Q_{N,n_0}^{SM} \approx Q^{TD},$$

where n_0 corresponds to a finite range of iterations of the RG transformation. It should be noticed that the values of Q_{N,n_0}^{SM} also approximate $\lim_{n \rightarrow \infty} \lim_{N \rightarrow \infty} Q^{SM}$, which represent the values of the given quantity after taking both the thermodynamic limit and the infinite iteration limit.

One might object that the results obtained in this section rely too much on an idealized case and that in actual practice things are more complicated. Although it is true that in practice things are less straightforward, numerical simulation gives an important support for what has been said here. Since 1976 there have been attempts to use the numerical Monte Carlo simulation in the framework of renormalization group methods for the study of critical exponents. The first contribution in this direction was made by Ma (1976), who suggested an application of real space RG methods that required the calculation of the renormalized Hamiltonians. However, since calculating the renormalized couplings accurately enough proved to be too difficult, this approach did not succeed in determining the fixed point Hamiltonian with significant precision. Pawley, Swendsen, and Wilson (1984) made further progress in this direction by suggesting an approach based on expectation values of the correlation functions that did not rely on the calculation of renormalized Hamiltonians. Using this approach, they showed that for an Ising square lattice with 64 number sites, the system approaches the behavior of an infinite system after two iterations of a RG transformation. After more iterations, however, the system was shown to depart from the expected results flowing towards a trivial fixed point. A plausible explanation for this cross-over was that after more iterations the correlation length became comparable to the size of the system and finitary effects became relevant.¹⁶

One should bear in mind, however, that for some models the convergence is not as rapid as for the 2D-Ising lattice. Therefore, in order to avoid finite size effects in the renormalized systems, one should use large lattices. In the past years there has been significant improvement in this direction. See, for example, Hsiao and Monceau (2002) and Itakura (2003).

6 Concluding Remarks

The arguments presented in this paper give us good reason to think that the appeal to the infinite limits in the theory of phase transitions does not represent a challenge for reduction, at least not for limiting reduction. In fact, contra what

¹⁶This is also pointed out by Butterfield (Butterfield, 2011, p. 69).

has been argued by Batterman (2001, 2009) and Morrison (2012), these arguments suggest that the infinities and divergences characteristic of the physics of phase transitions are not essential for giving an account of the phenomena since from finite statistical mechanics one can recover the thermodynamic behavior of phase transitions even in the case of continuous phase transitions, as it was shown in section 5.

Nevertheless, this does not mean that phase transitions are not inconsistent with other notions of reduction that have also been discussed in the philosophical literature. Norton (2013), for instance, correctly points out that the case of continuous phase transitions does not satisfy what he calls “few-many reduction”, according to which there will be a reduction if the behavior of a system with a few components can be used to explain the behavior of a system with a large number of them. The reason for this is that continuous phase transitions are intrinsically fluctuation phenomena that can only arise when N is sufficiently large.

Likewise, continuous phase transitions also seem to be at odds with the kind of reductive explanation that requires the explanans to give us accurate and detailed information about the microscopic causal mechanisms that produce the phenomenon (e.g. Kaplan (2011)). As it has been pointed out by Batterman (2002), Batterman and Rice (2014) and Morrison (2012), the impossibility of giving such an account is related with the robustness of the fixed point solutions under different choices of the initial conditions. This implies that the critical behavior is largely independent of specific microscopic details characterizing the different models and that the statistical mechanical account of phase transitions does not give us complete information about the microscopic mechanisms underlying the transitions. However, as it was shown in the paper, these senses in which reduction “fails” do not threaten the project of inter-theory reductionism in any relevant sense.

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