Master's Thesis in
Physics + Philosophy and Science Studies

Emergence and Phase Transitions

A Critical Investigation

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April 5, 2021

Abstract

This thesis seeks to examine the philosophical concept of emergence with respect to the particular case of phase transitions and whether the latter should be classified by the former. In investigating this, two relevant sub-questions are raised. First, to what extent and in which way do phase transitions fulfil the role of emergence. Second, can the concept of emergence be enlightened or informed by the case of phase transitions?

Emergence is a widely applied concept, but it lacks a universal meaning. In short emergence corresponds to a relation between a whole and its parts in which the whole is autonomous from its parts even if it depends on or arise from them. This is usually taken to mean that the whole cannot be predicted from, reduced to or explained by the parts and laws governing them.

It is observed that the topic of phase transitions alone has led to at least three partially independent approaches in which emergence is involved. At the phenomenological level phase transitions are observed as abrupt changes in matter leading to apparently qualitative changes in behaviour. Today they are more precisely described by physics, and in particular by the theories of thermodynamics, statistical mechanics and the renormalization group. The theory of thermodynamics defines these changes mathematically as discontinuities in the thermodynamic potential. One can show that the direct prediction of this discontinuity within the framework of statistical mechanics, is impossible without applying the thermodynamic limit, i.e., allowing for an infinite system of particles. Due to the incapability of the more fundamental and microscopic theory to predict them, phase transitions are by many considered as evidence for emergent behaviour. A second approach holds, in a more direct way, that phase transitions lead to emergent properties due to the apparently qualitative change in behaviour occurring after the transition. A third approach is related to the specific feature of universal behaviour associated with systems behaviour at critical points (where so-called critical or second order phase transitions take place). There microscopical distinct systems show identical macroscopic behaviour. These three are presented and critically investigated.

It is concluded that it is not clear whether the concept of emergence could be used to describe phase transitions in one or another way. It is argued that the example of phase transitions demonstrates that emergence often is imprecise in this task and that it could be replaced by other more nuanced concepts.

Preface

This thesis concludes my master degree in Physics + Philosophy and Science Studies at Roskilde University. It is an interdisciplinary thesis written within these two subjects. It was completed in April 2021.

I would like to thank my supervisor Martin Niss from the department of science and environment and my co-supervisor Patrick Blackburn from the department of communication and art. I am grateful for all the assistance and guidance during this project as well their contributions to interesting discussions. I would also like to thank my friends and family. Without their support, positivity and enthusiasm I wouldn't have been able to finish this project.

Contents

Chapter 1

Introduction

This thesis intends to combine the subject of philosophy and physics through a case study of phase transitions from a philosophical perspective. These phenomena, long known to the human observer and studied in depth by the physical sciences, have only recently been appreciated by philosophers. In contemporary literature they are sometimes seen as key examples of *emergence* (Bedau and Humphreys 2008, p.1), the particular philosophical concept that this thesisdeals with. It is common to associate this concept with the emergentist's aphorism stating that: "The whole is greater than the sum of its parts." (Silberstein and McGeever 1999, p.185). While the exact meaning of such a statement is far from unambiguous, it tends to be an appealing idea to a lot of people while simultaneously being subject to criticism. In the context of emergence it means something along the lines of cases at a certain level of complexity, where the whole, even though made up by smaller material parts, cannot be completely understood by these constituents alone. Today, this idea has gained wide popularity in philosophy, religion and art, but also in modern science. And a huge number of different phenomena are claimed to provide evidence supporting that emergent entities exist.

Ideas similar to or associated with the way emergence is used today relate back to at least Aristoteles, but in order to defend a specific philosophical position the term was first applied by Lewes in 1875 in connection with the so-called *British Emergentists* (O'Connor 2020). As a philosophical concept, emergence has most often appeared in the context of topics such as the philosophy of mind, artificial life and complex biological systems (Falkenburg and Morrison 2015, p.1). To argue that phenomena within the scope of physics could be emergent as well has in general been regarded as a more radical statement compared to the examples previously mentioned. This has to do with the fact that the explanations involved in physics generally (or traditionally) are expected to be in reductive terms. Almost without exception, every literature list belonging to a paper about emergence in physics includes Philip W. Anderson's very short, but still influential paper: *More Is Different* first published in 1972. This is the case despite the fact that the term 'emergent' or 'emergence' never appear in this paper.[1] Nevertheless, the ideas and arguments presented here may help to motivate for why emergence ought to be discussed also

[1]However he did apply it to condensed matter theory in (Anderson 2004).

in physics. The title suggests an alternative to the emergent aphorism mentioned above: the whole is not only more, but different from the sum of its parts (Anderson 2008, p.224). Particularly Anderson emphasises the sub-field of condensed matter physics, in which the the topic of phase transitions can be subsumed under, to exemplify cases where it is not possible or relevant to start from the smallest particles and reconstruct "everything" from that. In this context he states that:

> "*The constructionist hypothesis breaks down when confronted with the twin difficulties of scale and complexity. The behavior of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles.*" (Anderson 2008, p.222).

A few decades later, in *Why Is More Different - Philosophical Issues in Condensed Matter Physics and Complex Systems* (2015), the editors state about the field of condensed matter physics, that: "It is one of the few areas where physics and philosophy have a genuine overlap in terms of the questions that inform the debates about emergence." (Falkenburg and Morrison 2015, p.1).[2] One of the challenges involved in combining two subjects, is the task of making sure that the topic investigated claims a certain level of relevance to both subjects. It is my intention that the topics chosen for this thesis, phase transitions and emergence, together satisfy this aim.

1.1 Problem Formulation

The question I attempt to answer throughout the thesis is specified by the following problem formulation:

> *Should phase transitions be classified as emergent entities?*

In answering this, the goal is twofold:

1. To what extent and in which way do phase transitions fulfil the role of emergence?
2. Can the concept of emergence be enlightened or informed by the case of phase transitions?

The section below further elaborates and explains how these questions are to be understood. By this the scope of the thesis is determined.

[2]The term is also used by others in the context of other sub fields of physics such as quantum mechanics, quantum field theory, space-time theories and nonlinear dynamics but these are outside the scope of this thesis.

1.2 Methodology

The thesis is a theoretical study based on a selection of literature on the subject of emergence and phase transitions. The problem formulation, divided into two sub questions, should be understood as follows: The first question is the primary question. With respect to a pre-established concept or ideas relating to emergence the aim is to decide whether or to which extent emergence applies to phase transitions. In this sense, the thesis is a case study meaning that the conclusion made here is restricted to the specific case of phase transitions and cannot necessarily support any general conclusion about either emergence as concept and how it relates to other topics within physics or other subjects. However, it is observed in the literature about phase transitions that as an alternative to the strategy just described, some use this particular case, the study of phase transitions, to argue that emergence should be defined in a specific way.[3] This alternative should not be confused with how I answer the second question. I will not make my own definition of emergence based on this case study. Doing so would lead to circularity. The answers given to the first question, do however, I argue, show that the case study of phase transitions is able to illuminate the concept of emergence to a certain extent. To clarify this, is the aim of the second question. The section below elaborates on the steps involved.

1.3 Structure

The thesis contains four main chapters. The two first chapters intend to provide the theoretical background needed in philosophy and physics: Chapter (2) presents the term emergence from a philosophical perspective and chapter (3) introduces phase transitions as a topic in physics. Knowledge corresponding to undergraduate university level of thermodynamics and statistical mechanics is presupposed. As the theme of this thesis is phase transitions in a philosophical perspective, rigorous proofs or descriptions are omitted. Furthermore, chapter (4) looks at a selection of different approaches to the claim that phase transitions are emergent entities in the literature. The chapter is divided into three separated sections each presenting different arguments that introduce distinctive aspects and issues. These three chapters together enable for a final discussion in chapter (5) where the problem formulation is answered.

[3]This is not unique for this example and relates to the question about if scientific research and cases from actual sciences can affect or inform the way we define or understand emergence (or eventually other philosophical and theoretical terms). In its greater context, this furthermore relates to the distinction between philosophy of science that is either primary normative or descriptive.

Chapter 2

An Introduction to Emergence

As the introductory chapter briefly explained, emergence is a huge and widely applied subject, but it is also a quite complex topic. In this chapter the philosophical theory of emergence needed for the purpose of this thesis is presented. Emergence is defined in terms of the leading characteristics or core ideas that usually play a significant role when describing entities claimed to be denoted by this term. Additionally, familiar issues involved in determining the scope of emergence are addressed.

2.1 Defining Emergence

The concept of emergence does not have a definition in its strict sense. When reading the literature about emergence, one quickly discovers the variety of forms its description can take. Hence, whether or not it is used in a consistent way in the various of cases in which is claimed to apply to is not obvious. As a familiar fact, to be able to perform a conceptual analysis for evaluating which cases should be classified by a specific term and which ones that should not presupposes some necessary and sufficient criteria for what it means to be denoted by that term. This is exactly what is missing. That being said, the following sections attempt to formulate what emergence generally is about, remaining consistent with its traditional philosophical meaning, and aiming to provide a certain level of clarity, despite the missing unique definition.

2.1.1 Two Necessary Conditions: Autonomy and Dependence

To begin with consider the very first sentence introducing the term in the comprehensive book on the topic, *Emergence: Contemporary Readings in Philosophy and Science* (2008): "Emergence relates to phenomena that arise from and depend on some more basic phenomena yet are simultaneously autonomous from that base." (Bedau and Humphreys 2008, p.1). In the absence of a more specific definition, it seems fair to state that this sentence underlines what are the two necessary conditions involved in an emergent relation: namely the *autonomy* of what is claimed to be emergent as well as the *dependency*-relation to its base. For the sake of simplicity

I will henceforth use the terms "emergent entities" and "base entities" to denote and separate between them.[1]

At first glance, the conjunction of these two features, autonomy and dependence, might be an indication of an apparent contradiction. But alternatively, the conjunction of these two is what makes emergence attractive, as it can be classified as a position corresponding to somewhere in between the two extremes: hard *reductionism*[2] and versions of *dualism*[3] (O'Connor 2020). One way to understand this "middle way" is to think of emergence to be incorporated by the terms non-reductive physicalism or materialism (Kim 1999, p.4), maintaining that there is no doubt about the physical base in which the emergent entity arises from and depends on,[4] but that the complete knowledge of this base cannot provide all information about the emergent entity. Hence, emergent entities are autonomous in one way or another. (Kim 1999, p.7). However, this position, placed in the middle of two extremes, can result in an unstable position (Kim 1999, p.5).

2.1.2 The Scope of Emergence

Before elaborating what emergent relationships more specifically are about, consider the following questions as they may shed light on what kind of challenges that are involved in the process of understanding (and defining) the scope of emergence.

1. What classes of entities is it that emerges? Can it be phenomena, properties, processes, scientific laws, theories etc.?
2. Are there true cases of emergence meaning that there are actual emergent phenomena in nature compared to those entities that are emergent only relative to a given model or theoretical description?
3. If the term 'emergence' can be applied to different subjects as exemplified, does it need to or should it mean exactly the same in all cases?
4. Can emergence be a matter of degree? From weak to strong emergence?
5. Does it takes some time before the emergent entity appears? Is emergence static or a result of a dynamic process?

[1]The term 'entity' is picked here to keep it as general as possible. Which concrete terms that could eventually replace it differs from case to case. The question about the extension class of emergent entities is addressed below and throughout the thesis in general.

[2]Meaning the rejection for any sense of the autonomy of emergent entities. The general concept of reduction is more formally defined below.

[3]Meaning the rejection for any sense of the micro-dependence of the emergent entity. In philosophy dualism is more generally the claim that two distinct substances exist in the world and that they are independent of each other and hence none of them can affect or be affected by the other.

[4]Regarding the possibility of emergence in physics, the physical nature of the emergent entity is of course also never called in to question as it might be in some philosophical discussions about mental states for instance (Falkenburg and Morrison 2015, p.1).

Potential answers to these questions would affect whether emergence, if a feature of the world at all, is likely to be rare or common. A too strict idea about emergence could cause the difficulty of finding any actual examples satisfying it. If so, emergence would be a pure theoretical term probably lacking scientific interest. The opposite alternative could lead a too open or inclusive understanding of the term (Bedau and Humphreys 2008, p.12-13). While I will not provide definite answers to any of the questions raised above, the sections (2.1.3) and (2.1.4) furthermore describe the emergence concept.

2.1.3 Characteristics of Emergence

The strategy used when identifying emergent entities is usually pointing out the presence of one or several out of a set of typical characteristics. It is not clear whether or not it is sufficient to name an entity emergent if, for instance, only one of the the typical features is present it the particular case. Therefore, this way of defining a concept might be unsatisfactory; some favour or focus on only one of them while others see the importance of several of them (Bedau and Humphreys 2008, p.9). Due to this, it is perhaps better or more appropriate to use characteristics (hence the title of the this section) or even symptoms of emergence rather than conditions or criteria etc. However, such characteristics show different ways in which the autonomy of the emergent entities could be claimed while simultaneously emphasizing the dependence-relation to its physical base.

To define the characteristics of emergence in this thesis, I will refer to Kim (1999) in particular and what he calls "the central doctrines of emergence". The characteristics or doctrines in original form can be found in (Kim 1999, p.19-22) while a slightly different version is retrieved here:

1. Relation between Parts and Wholes [5]
2. Unpredictability
3. Irreducibility
4. Unexplainability[6]
5. New Causal Powers

The so-called doctrines of emergence appear in Kim's article *Making Sense of Emergence* in which the overall aim is to make the idea of emergence intelligible and to find a way to separate emergent entities from those that are *resultants* (Kim 1999, p.5), a distinction that is explained below and which Kim adopts from the classical emergentists.[7] Based on the literature on the topic of emergence it seems fair

[5]This term is meant to cover what Kim originally names the *emergence of complex higher-level entities* and the *emergence of higher level-properties*.

[6]In Kim's version *irreducibility* and *Unexplainability* are listed as the same point. The reason for why the two features are separated here is outlined below.

[7]Those that belonged to or are associated with the name *British emergentism* mentioned in the introduction. Kim is not necessarily himself a strong defender of emergence and he has argued against the idea elsewhere, but this is outside the scope of this thesis.

to state, and this is also what Kim asserts himself, that "the doctrines" together are consistent with the well-known idea of emergence/traditional philosophical view on emergence. As Kim points out, alternatives to these specific terms could have been chosen in stead, but those included on his list still, more or less, cover the same content as the alternatives (Kim 1999, p.20). Below I will make some independent comments to each of them elaborating how they are to be understood and interpreted in the context of emergence.

Relation between Parts and Wholes

The idea of emergence is strongly connected to the relation between complex wholes and the parts constituting them. Notice (by the citation introducing section (2.1.1) as well as the description given there) that the base entities in which the emergent entities depend on are usually taken to be the more *basic* entities. Generally, in the context of emergence (and reduction) the view that the world is organized into levels is normally presupposed, and furthermore it is assumed that what that emerges is located at a higher-level compared to what it emerges from. Hence some levels are taken to be either more or less fundamental than others resulting in an hierarchical structure of the world. Kim refers to this model as "the layered model". The early emergentists were among the first to articulate it more precisely (Kim 1999, p.19). A familiar example of this view on the world is to think of physics as more fundamental than chemistry being more fundamental than biology etc. Another example is that some level of description within physics itself is considered as more fundamental that another, e.g., statistical mechanics compared to thermodynamics. It is common to use the microscopic level and the macroscopic level as alternatives to denote such different "levels".[8] Another, idea that relates to the part-whole aspect of emergence is that of a higher-level of complexity of the whole. Entities with a higher level of complexity arise from the composition of the lower level entities which has resulted in new structural configurations or relations between them (Kim 1999, p.20). The terms *holism* or *holistic* are alternatively used.

What is important to point out is that although emergent entities are most likely to occur within this framework (set by the notion of the relation between parts and wholes and that they are higher-level complex entities), to claim the presence of emergence, more is required. This is due to that none of these aspects are unique to emergentism because neither are all complex entities emergent nor are all higher-level properties emergent. They could also be merely *resultants* (Kim 1999, p.20-21). In illustrating this difference, some examples may be helpful: consider for instance the concept of life and that of consciousness or mental states. Even though

[8] Emergence, at least the way it is intended to be understood and applied here, should be distinguished from for instance that phenomena belonging to different scales obey different fundamental laws as e.g. the theory of quantum mechanics at the atomic scale and the theory of general relativity at the cosmological scale (Falkenburg and Morrison 2015, p.1-2). This current understanding could of course change as a result of new discoveries and developments within the two or other theories. However, today the relationship between the level of cosmology and that of quantum mechanics is usually not claimed to be emergent and the theories describing the two subjects are inconsistent.

modern science presupposes that the world is made up by atoms, how exactly is it that these phenomena arise from the non-living entities? At least today, this "link" or relationship is not properly understood. An organism is in some sense just the molecules that constitute it, but at the same time, one cannot take the same set of molecules and reconstruct that organism (or any living organism). A similar description can be given about mental states, e.g, beliefs and desires. We expect them to depend on some biochemical and electrical activity in our brains, but still there is something autonomous about them (Bedau and Humphreys 2008, p.2). Compare these two cases to that of a house. If the house is decomposed into its smaller and different parts we are still able to rebuild it. Immediately, the last example seems not to be an example suitable to be identified by emergence, while the two former examples apparently may.[9]

The reason for why the house is not necessarily an appropriate example of emergence is that the house, even if one may describe it a complex composite of its material constituents, is not autonomous in the way that usually is required by emergentism. We can reduce it to its smaller parts (Morrison 2015, p.92).[10] In order to separate emergent entities from resultants at least one of the somehow commonly invoked, but still distinguishable features are usually claimed about emergent entities: namely that emergent entities are unpredictable from and/or irreducible and inexplicable to from their constituents parts.[11]

Unpredictability

The unpredictability of emergent entities means that one cannot predict them by the complete information of their basal conditions (or lower-level information) alone. This feature contrasts with resultant entities as they are predictable if this information is available (Kim 1999, p.21). Unpredictability is sometimes taken to be a consequence of irreducibility (Bedau and Humphreys 2008, p.10), see the next characteristic.

Irreducibility

In most cases emergence is contrasted with reduction and the failure of reduction is sometimes used alone as the hallmark of emergence. That being said, the relationship between reduction and emergence is complicated and someone alternatively holds that the two terms can be compatible.[12] The concept of reduction, although more frequently in use than emergence, also lacks a standard definition. In short, and in its simplest sense, irreduction, the way it is used to defend emergence, is just

[9]These examples are quite informal and I am not insisting on that all biologists today generally use the word emergence about life and living organisms, but I still think the difference the examples emphasizes can work to illustrate the point here.

[10]In Morrison (2015) the word *aggregate* is used in stead of resultant.

[11]Kim thinks that emergentists (meaning the British Emergentists) took the three to be be equivalent or at least to form a single package (Kim 1999, p.6). They are also likewise emphasized in (Falkenburg and Morrison 2015, p.1) and (Bedau and Humphreys 2008, p.9).

[12]This is for instance suggested about the example of phase transitions, see section (4.1.2).

that it is consistent with the the two claims of autonomy and dependence. (Bedau and Humphreys 2008, p.10). One version of reduction is known as *intertheoretic reduction* and due to the relevance that the relationship between the two theories of thermodynamics and statistical mechanics turns out to have for some of the points made in this thesis, it is worth focusing on this particular kind of reduction. The so-called Nagel-type of reduction (see Nagel 2013) is probably the most famous of this kind. It has been widely discussed and criticized[13] and different models of intertheoretic reduction are later being developed in different contexts, but it still tends to be what people has in mind when the term reduction is applied. Nagel makes it clear that it is not phenomena themselves that are reduced to other phenomena. Rather it is statements about them that are reduced to other statements (Nagel 2013), indicating the reductive relationship between two theories or at least statements about phenomena. It can be formulated by this general schema:

> *T reduces T' just in the case the laws of T' are derivable from those of T,*

where T' is the theory to be reduced from T'. (This definition is retrieved from Batterman (2020)). To find a pair of actual theories that directly fulfil this relation, which correspond to what Nagel named a *homogeneous reduction* has turned out to be rather difficult. One of the challenges involved is that the reduced theory might not always correspond to a subset of the reducing theory meaning that there may be concepts in the reduced theory not existing in the reducing theory. To make a way out of this Nagel defines a term *inhomogeneous reduction* which allows for moderations to the definition above. In short it is about defining some "bridge laws" or ways to connect concepts in the two theories to one another in cases where this is not obvious. This involves the permission to introduce some additional assumptions not appearing in the reducing theory. When this is done, then the concept or laws to be reduced must be derived from the reducing theory and the extra assumptions alone. The critique of this sense of reduction emphasizes the difficulty of deciding which additional assumptions that are legitimate and which that are not (O'Connor 2020).

Unexplainability

In the context of emergence, unexplainability is strongly related to both irreducibility and unpredictability and the presence of one of these two are often claimed to cause the a failure of explanation as well (see Bedau and Humphreys (2008) and Kim (1999)). I will not initially equate explanation with the failure of either prediction or reduction, since explanation is a topic on its own in the philosophical literature due to the different forms an explanation can take. As will become clear, the difference between explanations in general and reductive explanations has relevance for the example of phase transitions.

[13]Nagel himself was aware of many of the challenges involved.

New Causal Powers

New causal powers, *downward causation* or *top-down causation* are often claimed about emergent entities. In short it means that emergent entities have novel causal power not reducible to the causal powers of their basal constituents (Kim 1999, p.23). This feature is involved in the greater debate concerning causality or more specifically the question about what can be the possible directions of causation (being either same-level causation, upward causation or downward causation). While some argues that emergence fails to be an interesting concept without this feature, I will generally avoid discussions concerning causation as a characteristic on its own in order to limit the scope of this thesis. This choice, of course, leaves some fundamental philosophical questions unanswered, but I think it is possible to discuss emergence without taking a stand for or against this. This feature is sometimes claimed in connection with ontological emergence (Silberstein and McGeever 1999, p.182), defined below.

2.1.4 Different Versions of Emergence

In this chapter introducing emergence, I will finally describe some terms used to separate different possible ways an entity can be claimed to be emergent. These terms further illustrate the scope of emergence. One is the distinction between phenomena or properties in reality and the models or theories that we use when describing them usually known as *ontological* and *epistemological* emergence respectively. Furthermore, a way to separate between cases of emergence when time is involved and when is it not is given below under the names *synchronic* and *diachronic* emergence.

Epistemological and Ontological Emergence

The distinction between model and reality in this context could be concretized by the division between what is commonly referred to as epistemological and ontological emergence. This means for instance that one of the characteristics of emergence above, say irreducibility, may operate at either an epistemological level or an ontological level.

Of the two, epistemological emergence is generally thought of as the most likely version of emergence to occur. It claims novelty (or more precisely any other of the characteristics) only at a level of description. Epistemological emergence depends on theory and model choice (or options) or more generally, on our intellectual capacity at a given time. As emphasized above, while it is still true that the emergent entity, in terms of a higher-level description, depends on its base, it is very difficult or complicated for us to explain or derive the relevant properties or laws etc. from that base. Due to this description, epistemological emergence is artificial or at least it does not have any obvious ontological implications. The entity's status as emergent in this way can always be challenged, and hence potentially changed by the discovery of future models or theories (Silberstein and McGeever 1999, p. 182-186).

Ontological emergence is a stronger claim than epistemological emergence. It asserts, in contrast, that emergence or emergent entities really exist in nature. In Silberstein and McGeever (1999) it is further stated that: "By this we mean features of systems or wholes that possess causal capacities not reducible to any of the intrinsic causal capacities of the parts nor to any of the (reducible) relations between the parts." (Silberstein and McGeever 1999, p.185). The necessity of the last identification, between ontological emergence and causality, is is not hold by (Humphreys 2016). However, he holds that that ontological emergent features are objective and autonomous in that they do not depend on the state of knowledge of cognitive agents (Humphreys 2016, p.56).

To exemplify this distinction by a singe phenomenon, consider mental states. They could be thought of as epistemological emergent phenomena because we currently have no microscopic theory of the brain able to predict or explain them. Mental states could as well be thought of as ontologically emergent phenomena, if one believe that we will never be able to understand them with respect to their physical base. As mentioned, cases of epistemological emergence are more frequently identified. In contrast one may wonder whether it is realistic that there are cases of ontological or real emergence in nature. To show that an entity acquires status as ontologically emergent is the more difficult task as one then has to show that no possible shift in theory or description of the phenomenon is not, even in principle, able to challenge this status.

Synchronic and Diachronic Emergence

Another major division between accounts of emergence is the distinction between what is called synchronic and diachronic emergence. As epistemological and ontological emergence, this division illustrate the scope of emergence, see e.g. Humphereys (2016) and Bedau and Humphreys (2008). The main difference between synchronic (or static) and diachronic (or dynamic) emergence, is that the former corresponds to a relationship in which the emergent feature exists simultaneously as the base it emerges from while in contrast, diachronic emergence is used when the emergent feature appears over time. This means that it takes some time for the emergent feature to appear from the base it arises from. While not exclusively, the synchronic type of emergence is exemplified in cases where emergence is thought of as a relationship between a lower and a higher-level theory. The philosophical literature has mainly been concerned with this aspect.The use of the diachronic type of emergence is more likely to be observed within some approaches to emergence in modern science. Examples hereof are complexity theory and artificial life (Bedau and Humphreys 2008, p.5, 341).

Humphreys (2016) particularly criticizes the philosophical literature for favouring the synchronic versions of emergence which according to him excludes many physical systems which involve horizontal processes in time (Humphreys 2016, p.3). Humphreys claims that emergence is relational meaning that the emergent entities must result from (and hence depend on) something else, but allows for that, in some versions of emergence, the relation can be symmetric (Humphreys 2016, p.28-29).[14] In other words, the emergent entities and its base entities can be at at the same "level" or horizontal rather than the vertical structure emphasized in Kim's description of the parts and whole relation in section (2.1.3). Synchronic and diachronic emergence might be combined with epistemological and ontological emergence.

2.2 Summary

There is no single definition being able to uniquely determining the scope of emergence. However, emergence requires the simultaneous presence of autonomy and dependence meaning that the emergent entities are autonomous even though the arise from and hence depends on their physical base. Further, these conditions can be specified different characteristics or leading ideas of emergence. In this thesis, Kim's "central doctrines of emergence" are used for this purpose. First, emergence is (usually) a part and whole-relation (sometimes corresponding to a higher-level description and a lower-level description). What distinguish emergent entities from those wholes being resultants are that they are unpredictable from, irreducible to and inexplicable by its parts or constituents. Additionally, these characteristics may operate in different ways depending on whether the emergent entity is claimed to be a real phenomena in nature or emergent only relative to a theory for instance, corresponding to the notion ontological emergence and epistemological emergence respectively. In addition one may separate between what is called synchronic and diachronic emergence. Synchronic emergence was originally favored by the philosophical literature while diachronic emergence more often are recognized in descriptions in modern science. Horizontal versions of diachronic emergence challenges the view that emergence is a relation between parts and wholes. Whether these concepts apply to phase transitions or not will be discussed in chapter (5).

[14]An emergent symmetric relation means that an entities of type A may emerge from entities of type B and an entities of type B emerges can emerge from entities of type A.

Chapter 3

The Theory of Phase Transitions

This chapter is an introduction to the theory of phase transitions. Today, the subject of phase transitions are described by three different theories, or more generally theoretical frameworks. These are thermodynamics, statistical mechanics and the renormalization group. A basic level of knowledge of the two first subjects is presupposed. The first section is a short description of the relationship between thermodynamics and statistical mechanics. The second section is a general introduction to phase transitions as it is treated by thermodynamics. The third section aims (mainly) to explain in some technical details what will be referred to as the "problem of phase transitions" in statistical mechanics.[1] This "problem" is one of the main reasons for why phase transitions are regarded as relevant to be investigated with respect to emergence. The so-called *thermodynamic limit* plays a crucial role in this context. The section about statistical mechanics is concluded by a "second" problem which not directly connects to emergence in this thesis, but serves as motivation for why the renormalization group was needed in the first place, the topic of the fourth section. A conceptual or qualitative description of the renormalization group is provided. This theoretical framework plays a crucial role in several subfields of physics today, but in the context of phase transitions, the renormalization group is involved in the description of *critical phenomena* and *universality*.

The reader should be informed about that some of the details contained in the theory presented in this chapter are not by themselves necessary for the philosophical purpose of the thesis. These details are still included here according to an aim of providing a basic, but still sufficient, introduction to the theories involved in describing phase transitions.

3.1 The Relationship Between Thermodynamics and Statistical Mechanics

Thermodynamics, the older theory and statistical mechanics, the newer theory, both deal with thermal systems. A thermal system typically consists of a large number of particles in the order of magnitude 10^{23}. A system described by thermodynamics

[1]The name is adopted from (Liu 1999, p.97).

is macroscopic. It is identified by thermodynamic parameters such as pressure (P), temperature (T), and magnetic field (B) in which all can be obtained experimentally. Thermodynamics is a phenomenological theory of matter meaning that its fundamental concepts are drawn directly from experiments. While the laws or theoretical statements it introduces match the observed macroscopic experience of the physical world, the theory does not provide a deeper understanding of the physical details of the systems (Huang 1963, p.3-7). In this thesis equilibrium states are presupposed. When the parameters mentioned above do not change in time, one says that the system is in thermodynamic equilibrium (Huang 1963, p.3). The aim of statistical mechanics is to derive the thermodynamic equilibrium properties of a macroscopic system from the laws of molecular dynamics. Even though it is a microscopic theory, statistical mechanics still (of course) does not study the behaviour of each single particle involved. Rather it studies the most probable distribution of the collection of particles. The system under consideration is modelled by a suitable statistical ensemble and the thermodynamic properties are to be obtained by the corresponding partition function. Despite the theory's ability to state the specific equilibrium state for a given system, the theory cannot describe how this system approaches equilibrium or whether or not it can be found to be in a state of equilibrium in general (Huang 1963, p.139-140).

Many philosophers of physics and physicists themselves have investigated the relationship between these two theories and the claim that thermodynamics is the macroscopic, or less fundamental, theory compared to statistical mechanics as the more fundamental, underlying, microscopic theory. In the philosophical literature this relationship is sometimes taken to be the primary, well understood example of intertheoretic reduction (explained in section(2.1.3)) in which the former reduces to the latter. While it is true that the tools of statistical mechanics has been successful in explaining the concepts of thermodynamics and also why these concepts work as well as they do, the relationship is, at least at the conceptual level, complicated. For instance, it is not always obvious in exactly which way a term in the older theory should be connected to terms in the newer theory. An example hereof is entropy, corresponding to a single term in thermodynamics, but several terms in statistical mechanics (Sklar 2015). Another more general aspect to point to is the fact that statistical mechanics is a probabilistic theory and thermodynamics is not.

Among the numbers of examples that could have been examined is the phenomenon of phase transitions. The main relevance for this thesis relates to the question about whether the definition of phase transitions given by thermodynamics can be reproduced within the framework of statistical mechanics or not. In order to see why this is so, we need to ask the question: What are phase transitions according to these two theories?

3.2 The Thermodynamic Description of Phase Transitions

In the physical sciences, a phase corresponds to a subsystem or region in which all physical properties of a material are homogeneous. A phase of matter can be characterized by possessing a specific structure and symmetry. Phases of matter do not only include ordinary materials being in its either solid, liquid or gas phase,[2] but also e.g., a variety of magnetic materials which can change from the paramagnetic to the ferromagnetic phase when heated. The different phases are stable under different conditions and correspond to minima in the free energy. Going from one phase to another in these cases is for obvious reasons referred to as going through a phase transition. The process of a phase transition, does often, but not always involve a break in symmetry (Kadanoff 2013a, p.10).

3.2.1 The Definition of Phase Transitions

Physically or phenomenologically, one may say that a phase transition is observed as an abrupt or qualitative change in the behaviour of a system (Kadanoff 2000, p.209). More formally and according to classical thermodynamics, a phase transition is defined (mathematically) as follows:

Definition 1 *A phase transition is identified by a singularity or a discontinuity in the derivatives of the thermodynamic potential (or free energy).* (Callender and Menon 2013, p.194).

Phase transitions, as we know them from our everyday life, e.g., melting ice or boiling water, are so-called *first order* phase transitions. This kind of phase transition is called a *discontinuous* phase transition, since the discontinuity is to be found in the first derivative of the thermodynamic potential or equation of state. More generally an n'th order phase transition is a discontinuity in the n'th order derivative. Hence, higher order phase transitions are continuous in their first derivative and are therefore together named *continuous* phase transitions (Callender and Menon 2013, p.191-192). The *second order* phase transitions are the only ones, beside the first order transitions, that exist in nature as far as we know. They are identified by being continuous in the first derivative, but exhibiting a discontinuity in the second derivative. The transition from paramagnetism to ferromagnetism mentioned above is an example of a second order phase transition. Second order phase transitions take place at the so-called *critical point* (critical temperature and pressure) and are in modern language more commonly referred to as critical phase transitions (Kadanoff 2000, p.211).

[2] Or subphases of these.

3.2.2 The Fluid System

Before going further with the thermodynamic definition of phase transitions and the problems it implies in statistical mechanics, some illustrations and related concepts may be helpful. It is possible to show that different fluid and magnetic systems can be modelled mathematically in an analogous way. In this thesis the theoretical description of phase transitions focuses mainly on fluid systems.[3]

The thermodynamic parameters pressure (P), density (ρ) and temperature (T) or eventually P, volume (V) and T and the relations between them can be used to describe a fluid system at its basic level. The relation between them through the equation of state:

$$f(P, \rho, T) = 0 \tag{3.1}$$

defines a three-dimensional surface in which each point of the surface corresponds to an equilibrium state of the system. Information of the fluid system can easier be obtained by its projections on the three separated two dimensional planes. Figures (3.1a-3.1c) show the graphic representations of these three planes.

Consider Figure (3.1a) representing the PT-plane. The pure solid, liquid and gaseous phases are separated by the thick lines. Along these lines two phases can coexist, e.g., at the fusion curve. This is where the phase transition between the solid and liquid phase takes place, or more generally, along these lines the system is undergoing a first order phase transition. At the *triple point* in the diagram, all three phases can coexist. At the *critical point* (T_c, P_c) (or (T_c, ρ_c, P_c) in three dimensions), marking the end of the line separating the liquid and gaseous phase, the second order phase transition takes place. At and above this point, there is no longer any fundamental difference between the liquid and gaseous phases because the the difference in density between them is zero here. The difference in densities between the two phases of a particular fluid is an essential parameter named the *order parameter*:

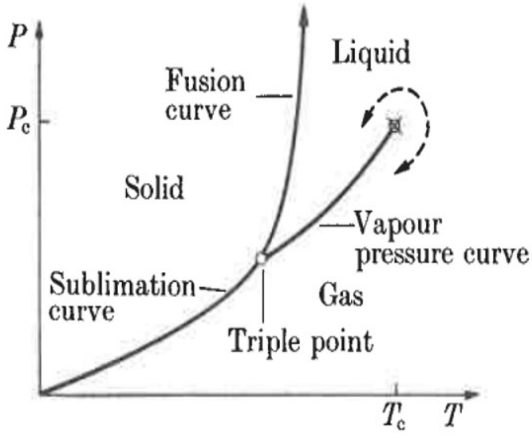
$$\Psi = |\rho_{liq} - \rho_{gas}| \tag{3.2}$$

Below the critical point this is a non-zero value. Approaching the critical point this value gets smaller and smaller before it vanishes above that point.[4] This behaviour is better illustrated in the phase diagram obtained by the $T\rho$-plane, see Figure (3.1c). The coexistence curve of liquid and gas for a fluid is shown here. We observe that the difference in density between the two phases disappears at the critical point (Stanely 1971, pp. 1–4). No such "end point" is so far found on the fusion curve in Figure (3.1a).

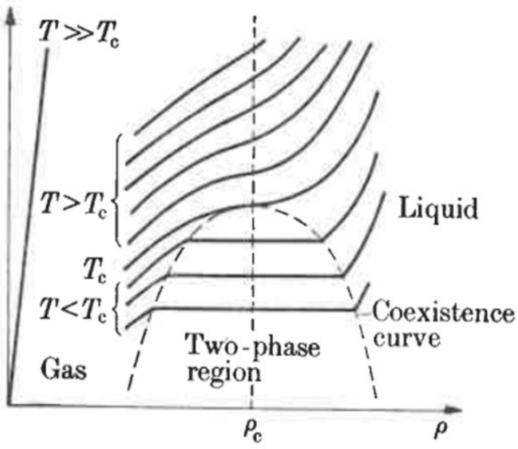
Regarding Figure (3.1b) isotherms corresponding to increasing temperatures are drawn in the ρP-plane. Also here, the qualitative difference between first and second order transitions can be observed. As the critical temperature is reached, the discontinuity at the first order transition between the gaseous and the liquid phase

[3]See Stanely (1971) for a more complete description of this analogy.

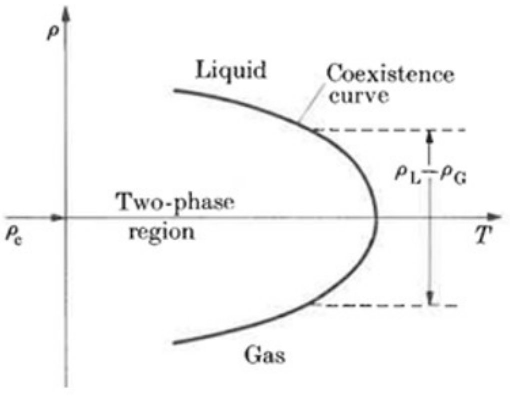
[4]A quantity that changes at the critical point such that it is non-zero before and zero above it, is a common feature for several physical systems and generally named order parameter.



(a) Temperature versus pressure.



(b) Density versus pressure.



(c) Temperature versus density.

Figure 3.1: The figures are retrieved from (Stanely 1971, p.3-5).

is no longer present and the isotherms for all temperatures above this temperature are continuous.

Another relevant parameter, named the *reduced temperature* is defined as follows:

$$t = \left| \frac{T - T_C}{T_C} \right| \tag{3.3}$$

It is a dimensionless quantity telling the difference in temperature from the system at criticality. Note that $\epsilon = 0$ at the critical point since $T = T_C$. Close to the critical point the order parameter becomes proportional to a power of the reduced temperature:

$$\Psi = |\rho_{liq} - \rho_{gas}| \propto | - t|^{\beta} \tag{3.4}$$

We see that the discontinuous jump in the order parameter identifying the first order transition goes to zero with the power of β as the critical point is approached (Kadanoff 2013b, p.162). β is one out of several so-called *critical exponents* characterising the critical behaviour of the system. The importance of these parameters will be elaborated in section (3.4) where some of the tools of the renormalization group are described.

3.3 Statistical Mechanics and The Problem of Phase Transitions

We continue by relating statistical mechanics to the definition of phase transitions in thermodynamics above. By this we approach the core of the problem connected to phase transitions in statistical mechanics. The problem, to be outlined just below, is from now on referred to as "the problem of phase transitions" in the rest of the thesis.

3.3.1 The Problem Outlined

A phase transition, the way it is defined in thermodynamics (see Definition 1) is not possible in a finite system in statistical mechanics or, as we will see, unless one applies the so-called *thermodynamic limit.* In the thermodynamic limit the number of particles in the system and the volume go to infinity, keeping the density fixed (Callender and Menon 2013, p.195):

$$N \to \infty, \qquad V \to \infty, \qquad \frac{N}{V} = \text{constant.} \tag{3.5}$$

In reality a thermal system is composed of a large number of molecules and hence the volume occupied by them is correspondingly large. The typical order of magnitude of N and V is, as mentioned above, 10^{23} molecules and 10^{23} molecular volumes respectively (Huang 1963, p.140). However, even though these are great numbers, the subject of physics and the systems we want to describe, consist of a finite number of particles, so the infinity involved is at least a potential conceptual problem (see section (4.1)).

The problem of defining phase transitions in statistical mechanics for finite systems is of mathematical character. It has been common to visualize it through what one may name the “Lee and Yang approach/solution” to the problem. Their work includes two important theorems and results derived from them (see next section). Before going through their method in details, a summary of the (mathematical) problem may be outlined as follows:

1. In statistical mechanics, the free energy (associated with the different statistical ensembles) is defined in terms of the logarithm of the partition function, Z (the equation of state includes a term like that).

2. In order to obtain a singularity in this function, the roots of the partition function, Z, can be calculated (because the logarithm function exhibits a singularity as its argument goes to zero).

3. But the equation $Z = 0$ does not have any real and positive solutions (required to make sense in physics) as long as the system remains finite.

The connections between (1), (2) and (3) as well as why they hold is explained below.

3.3.2 The Theory of Lee and Yang

In *Statistical Theory of Equations of State and Phase Transitions. 1. Theory of Condensation* (1952), Lee and Yang study the behaviour of a non-ideal monoatomic gas in statistical mechanics. They conclude that: “The study of the equations of state and phase transitions can thus be reduced to the investigation of the distribution of roots of the grand partition function.” (Lee and Yang 1952a, p.406). The following is a review of their research leading to this conclusion. However, the review is written with the aid of Huang (1963) and Liu (1999), not necessarily identical to the original version, but the results are equivalent with those obtained in Lee and Yang (1952a). One starts by defining a statistical ensemble, for instance the grand canonical ensemble, where the number of particles, N is allowed to be interchanged, but the temperature, T, volume, V and chemical potential, μ, are kept constant. Once the partition function, $Z_G(V, T, \mu)$ is known, one is able to calculate different thermodynamic properties. For the partition function to be obtained, the Hamilitonian must be known and hence knowledge about the interaction between the particles in the monoatomic gas must be specified. Consider particles of size (diameter) equal to a and that they are impenetrable. The distance between particle i and j is r_{ij}. Further, the length in which there is an interaction between two particles has an upper limit, r_0. Then the interaction defined as the potential $u(r_{ij})$ between particle i and j, may be defined as:

- $u(r) = \infty$ for $r \leq a$
- $0 < u(r) < -\epsilon$ for $a < r < r_0$
- $u(r) = 0$ for $r \geq r_0$

The corresponding Hamiltonian, H, for the system is then the sum of its potential energy, U, and its kinetic energy, K, in three dimensions expressed as:

$$K = \sum_{i=1}^{3N} \frac{p_i^2}{2m} \tag{3.6}$$

$$U = \sum_{i<j}^{N} u(r_{ij}) \tag{3.7}$$

The Boltzmann factor for the grand canonical ensemble is:

$$e^{-\beta(H-\mu N)} \tag{3.8}$$

where $\beta = k_b T$ and μ is the chemical potential. Hence, the total partition function for the system takes the form:

$$Z_G(V,T,\mu) = \sum_{N=0}^{N_{max}} \sum_{i=1}^{N} e^{-\beta(H_i-\mu N)} \tag{3.9}$$

For the purpose of what we want to show, it is advantageous to observe that equation (3.9) may be written as a polynomial of the fugacity, $z = e^{\beta\mu}$, with coefficients $Q_N = \sum_{i=1}^{N} e^{-\beta H_i}$. Applying such substitutions equation (3.9) may be written as:

$$Z_G(z,V,T) = \sum_{N=0}^{N_{max}} Q_N z^N = 1 + Q_1 z + Q_2 z^2 + ... + Q_{N_{max}} z^{N_{max}} \tag{3.10}$$

The corresponding equation of state is defined as:

$$p = \frac{1}{\beta V} \lg(Z_G) \tag{3.11}$$

$$\frac{1}{v} = \frac{1}{V} z \frac{\partial}{\partial z} \frac{1}{V} \lg(Z_G) \tag{3.12}$$

where p is the pressure and $v = \frac{V}{N}$ = *specific volume*. We observe from equation (3.10) that the coefficients of Z_G (a polynomial of finite degree, N_{max}) all are positive by definition.[5] This leads to the result that none of the roots of this polynomial, or the solution to the equation $Z_G = 0$, can be real and positive. Therefore, for any finite volume, phase transitions, defined as non-analytical behaviour in the equation of state, cannot be identified.

[5]The exponential function is always > 0.

The Need for the Thermodynamic Limit

Approaching the mathematical problem above, the following limits or limit quantities may be considered (meaning that we are studying p and $\frac{1}{v}$ in the thermodynamic limit):

$$p = \lim_{V\to\infty} \frac{1}{\beta V} \lg(Z_G) \tag{3.13}$$

$$\frac{1}{v} = \lim_{V\to\infty} z\frac{\partial}{\partial z}\frac{1}{V} \lg(Z_G) \tag{3.14}$$

In the article cited above, Lee and Yang intend to show that:

- These limits exists: (3.13) and (3.14).
- The correct equations of state are (3.13) and (3.14), that is, they describe both gas and condensed phases.
- Singularities (may) appear at the thermodynamic limit, that is, as V approaches infinity, some of the roots may converge towards the positive real axis. Hence phase transitions can be identified within the framework of statistical mechanics.

As already mentioned, in order to fulfill what is stated here, two theorems are needed and proved.[6] The theorems state the following:

THEOREM 1 For all positive real values of z, $\frac{1}{V}\lg(Z_G)$ approaches, as $V \to \infty$, a limit which is a continuous, monotonically increasing function of z, independent of the shape of V. In other words, the limit exists.[7]

THEOREM 2 If in the complex z plane a region R containing a segment of the positive real axis is always free of roots, then in this region as $V \to \infty$, for all z, $\frac{1}{V}\lg(Z_G)$ converges uniformly to a limit which is an analytic function.

Important consequences are to be obtained from these two theorems. The regions R in the complex plane z from Theorem 2, may be thought of as corresponding to single homogeneous phases of the system. We may define a quantity p_∞:

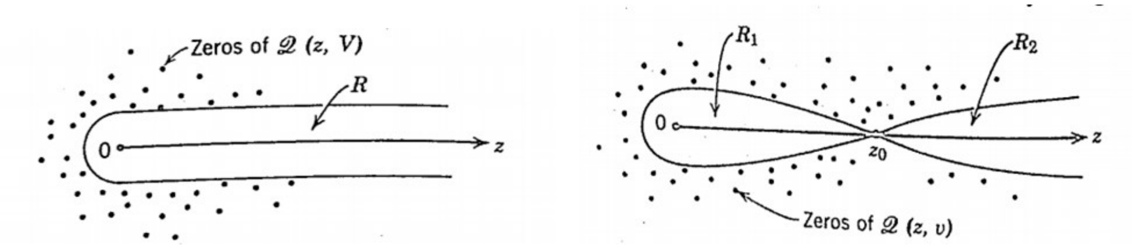
$$p_\infty = \lim_{V\to\infty} \frac{1}{\beta V} \lg(Z_G) \tag{3.15}$$

We know that this converges uniformly in any single phase in this limit. As a consequence of this, $\frac{\partial}{\partial z}$ and $\lim_{V\to\infty}$ commute in R, that is, the order of two can be interchanged so that in any single phase, one obtains:

$$\lim_{V\to\infty} z\frac{\partial}{\partial z}\frac{1}{V} \lg(Z_G) = z\frac{\partial}{\partial z}\frac{1}{V}\lim_{V\to\infty} \lg(Z_G) \tag{3.16}$$

[6]The theorems are not proved here, but the proofs but can be found in (Lee and Yang 1952a, p.408-409).

[7]Additional assumption: the shape of V is not so queer that its surface area increases faster than $V^{\frac{2}{3}}$.



(a) CASE 1 illustrated.

(b) CASE 2 illustrated.

Figure 3.2: The figures are retrieved from (Huang 1963, p.318).

From this, together with equation (3.13) and (3.14) we may define a quantity, a relation between the inverted specific volume and the pressure and in this limit:

$$\frac{1}{v} = z\frac{\partial}{\partial z}\beta p_\infty \tag{3.17}$$

Some examples considering different forms of the regions R from Theorem 2, may be illustrative regarding possible behaviour of the equation of state. The examples are retrieved from Lee and Yang (1952a) and Huang (1963):

CASE 1 There exists a region R which contains the whole positive real axis and is free of roots/ the solution of $Z_G = 0$ includes no positive, real roots as $V \to \infty$. Applying the two theorems in this case, leads to that both the pressure and the density are analytical in this region, and hence there cannot be any phase transition. The region corresponds to a single phase. See Figure (3.2a).

CASE 2 There is a point on the real y-axis (a zero), which Z_G approaches, as $V \to \infty$. As a consequence of Theorem 1, the pressure must be continuous, but the "density"/ inverted specific volume, as its first derivative (see equation (3.17)), may be discontinuous - which, eventually, corresponds to a first order phase transition. See Figure (3.2b).

Concluding this section, it is emphasized that there are actual problems in statistical mechanics where the theory described above is applied and phase transitions, understood as non-analyticities, are confirmed. This is possible for the two dimensional Ising model. The relevant equation $Z_G = 0$ have solutions distributed at the unit circle in the complex plane. As $V \to \infty$, the distribution becomes denser and denser and eventually one of the roots will be at the intersection between the positive real axis and the unit circle. This can be formulated by another theorem (Lee and Yang 1952b, p.414) stating that:

THEOREM 3 If the interaction between the atoms is as described above, then all the roots of the polynomial lie on the unit circle in the complex plane.

This example, the application to the two dimensional Ising model, shows that the theory given here is valid for (at least) one concrete mathematical problem (Huang 1963, p.320). A detailed calculation of this, applied both to the lattice gas model and a magnetic system is to be found in Lee and Yang (1952b).

3.3.3 A Second Problem: The Failure of Mean Field Theory

Beside "the problem of phase transitions", there was another separate problem involved the statistical mechanical treatment of phase transitions. This is connected to what is known as *mean field theory*,[8] an approximate theory which was the dominant approach to statistical mechanics before the development of the renormalization group (see next section). The theory is capable to provide a qualitatively correct description of the physics of phase transitions in some cases. But for many purposes, however, it has been replaced by the renormalization group and this is due to that mean field theory introduces an approximation which only succeeds in describing systems away from their critical points (Kadanoff 2013b, p.162).[9] To explain this, consider the two dimensional Ising model mentioned above. The Ising model was originally developed to describe the magnetic system (or the Ising ferromagnet) (Kadanoff 2013a, p.17), but a model equivalent to that one can be applied in the case of the fluid system as well, the lattice-gas model. In order to keep consistency with the rest of this theoretical description, we continue by the fluid system. However, both systems can be modelled by a two dimensional lattice consisting of cells in which each cell is given a particular value corresponding to a particular state of the system. In the liquid-gas system we may name this cell variable e_i and define it so that:

$$e_i = \begin{cases} 1 & \text{if cell } i \text{ is occupied by a particle,} \\ \\ 0 & \text{if cell } i \text{ is empty.} \end{cases} \tag{3.18}$$

The distribution of "1's" in the lattice corresponds to the local density of the fluid. Recall the short-ranged interaction between two particles, $u(r_{ij})$, in section (3.3.2). Figure (3.3) is a visualization of one particular example of the model. For the simplest Ising model we suppose that this interaction is restricted to a nearest-neighbour interaction so that:

$$u(r_{ij}) = \begin{cases} \infty \quad \text{if} \quad r_{ij} = 0, \\ \\ -\epsilon_0 \quad \text{if} \quad i \quad \text{and} \quad j \quad \text{are neighbouring cells and both are occupied,} \\ \\ 0 \quad \text{otherwise.} \end{cases} \tag{3.19}$$

[8]The term 'mean field theory' refers to a cluster of several slightly different so-called mean field theories. In 1937 Landau provided a general framework that generalized some of the previous mean field theories of phase transitions (Kadanoff 2013b, p.144).

[9]Mean field theory *is* reliable near critical points for systems of dimension greater than four (Kadanoff 2000, p.243), but if the aim is to study real systems, these systems are of less importance.

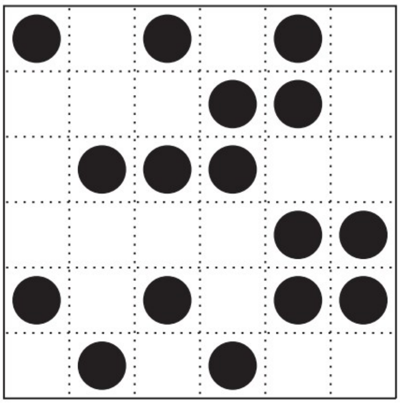


Figure 3.3: A visualization of the two dimensional lattice representation of the fluid. The black circles represent particles. The figure is retrieved from (Friedli and Velenik 2018, p.28).

The idea is that the these local interactions in sum, represent the long-range interactions characteristic for a thermodynamic phase (Callender and Menon 2013, p.194).

We now return to the approximation made in mean field theory, mentioned above. As known, in statistical mechanics, the different thermodynamic functions characterizing a particular system are all obtained from the system's partition function. To perform calculations of a system consisting of a lot of cells, the partition function alone becomes an intractable problem when the number of particles is large. This is due to the couplings between the (neighbouring) particles in the system's Hamiltonian. Therefore, mean field theory makes the assumption that each cell is affected by the mean field only (Callender and Menon 2013, p.194). In other words, each occupied cell (or particle) acts as if it was an independent one meaning that the sum of the particular neighbouring influence are replaced by the average behavior or the mean field produced by all other particles in the lattice. (Kadanoff 2000, p.215, 226). This results in that fluctuations away from this average value are ignored. In situations where fluctuations actually dominate the effect of the average behaviour or mean value, the approximation becomes unsatisfactory and mean field theory must be considered as the wrong approach (Kadanoff 2000, p.242). And it turns out that as one approaches the critical point the role of the fluctuations become important. And at the critical point the *correlation length*, ξ, diverges. The correlation length is the length defining the distance in which the particles can interact with one another. If the correlation length increases, more particles will interact, meaning that degrees of freedom are coupled together, then fluctuations away from the middle value can no longer be neglected. As a direct consequence, the mean field theory fails to predict the value of the critical exponents that matches experimental data. For instance, the theoretical value of β in equation (3.4) is in mean field theory predicted to be 0.5 while the measured experimental value is 0.32. Hence, new theoretical tools are needed (Callender and Menon 2013, p.193-194).

Notice that the failure of mean field theory at critical points takes place *even* in the thermodynamic limit, so this is an distinctive issue from the conceptual issue introduced by "the problem of phase transitions". It is both the disagreement with experimental results and theoretical contradictions that motivated for alternatives to the mean field approach (see Kadanoff 2013b, p.164-167).

3.4 Phase Transitions and The Renormalization Group

The renormalization group was originally developed in the field of particle physics. As mean field theory, it is not a theory in itself. Rather, it is a method of analysis which is used as a tool or theoretical framework in connection with statistical mechanics.[10] As my knowledge of this subject is limited, the intention of this section is not to provide a complete description of the renormalization group involving calculations. Rather it is to offer the general idea of the advantages and results of this technique in the context of phase transitions. There the renormalization group is needed for at least two different purposes: One is to predict critical behavior of particular systems and the other is to explain the universal behaviour which apply to classes of systems. The thermodynamic limit is required for both purposes (Callender and Menon 2013, p.218).

3.4.1 Critical Phenomena and Universality - A Renormalization Group Account

Critical phenomena, refers to the behavior of systems at their critical point i.e., point of second order phase transition. This behaviour is expressed in terms of several critical exponents, see Figure (3.4). In contrast to mean field theory, the techniques of the renormalization group is able to predict these values obtaining a much higher precision compared to the experimental values. Some systems show the same critical behaviour, a fact which is named *universality*.[11] Furthermore: "The set of all systems which have a given critical behaviour is called *universality class*." (Kadanoff 2000, p.248).[12] The systems that belong to the same universality class will under the renormalization scaling transformation on the space of Hamiltonians, flow to the same so-called *fixed point* (see below). These systems are originally described by different microscopical details, represented by their respective Hamiltonian func-

[10]The techniques of the renormalization group differs in a substantial way from traditional statistical mechanics including mean field theory, as the latter restricts it self to tools being orthodox in statistical mechanics. In short: While statistical mechanics (and mean field theory) uses a statistical ensemble (defined by a Hamiltonian) to calculate an average, in the renormalization group you calculate a another ensemble from the original statistical ensemble. It describes how things change under transformation and is more linked to the mathematics of "dynamical system theory" than probability theory (Kadanoff 2013b, p.180). Due to this difference, even if the renormalization group is used in connection with statistical mechanics, it gets its own section.

[11]This is not just a theoretical artifact (Kadanoff 2013b, p.178), see Lee and Yang (1952b).

[12]It does not follow from this that the values of their critical points (critical temperature and critical pressure) are identical. Actually, these values differ from system to system.

Values of selected Critical Exponents				
Exponent	Variable	Landau Values	Ising $d = 2$	Ising $d = 3$
α	Heat Capacity	0	0	0.12
β	Order Parameter	$\frac{1}{2}$	$\frac{1}{8}$	0.31
γ	Response Function	1	$\frac{7}{4}$	1.25
δ	Critical Isotherm	3	15	5.20
ν	Correlation Length	$\frac{1}{2}$	1	0.64
η	Pair correlation at T_c	0	$\frac{1}{4}$	0.06

Figure 3.4: Some of the critical exponents. The figure is retrieved from (Mainwood 2006, p.150).

tion. For instance the transition between paramagnetism and ferromagnetism and the liquid-gas transition (including different fluid systems) at the critical point correspond to the same universal class. The analysis provided by the renormalization group shows that some of the details describing and distinguishing systems from one another are irrelevant for the universal behaviour at critical points, while simultaneously determining those details that are important for this specific behaviour. Examples of the latter are the spatial dimension of the system and symmetry properties of the order parameter (Batterman 2002, p.42).

The Method

In order to explain how the method of the renormalization group works for the purposes just mentioned consider the two dimensional Ising model again. Different approaches exist but the one to be explained below is so-called real-space renormalization in which its central idea is originating from Kadanoff (Mainwood 2006, p.153). In general one performs a coarse-graining procedure on the lattice system which can be thought of as a transformation, τ, in the Hamiltonian describing the system. Or you could say a transformation in the coupling parameter since the Hamiltonian is characterized by the coupling strength between the atoms. The characteristic length of a system refers to the spatial distance between correlated blocks or cites in the Ising model, e.g., the space between the positions of the atoms. As already emphasized, usually, the molecules in a gas or a liquid interact weakly with one another (short range forces), meaning that one molecule is only significantly correlated with its other nearby molecules. This would imply a short correlation length. But as the temperature increases towards the critical temperature, the correlation length increases. As mentioned, the length is found to diverge at the critical point meaning that the system has no characteristic length scale at this point. Since a lot of atoms or components of degrees of freedom are coupled together, the mathematical problem becomes intractable or practically impossible to solve. One of the advantages of the renormalization group is that it can be used to turn the initially intractable problem to another more tractable problem (Batterman 2010, p.1042).

The scaling transformation of the parameter space of Hamiltonians, which maps an original problem to another at a different scale, is made so that it preserves all the large-scale properties of the system (Mainwood 2006, p.153). It can be summarized by three steps illustrated in Figure (3.5):

a) Reducing

b) Rescaling

c) Renormalizion

The lattice shown in the figure can be used to model either a fluid system or a magnet system. In the first case, each cell would correspond the presence of a molecule or not.The first step (a) is about forming "blocks" of a certain number of cells, in this case blocks of size four. These four are then replaced by a new variable representing the value of sum of the old blocks. This reduces the degrees of freedom coupled to one another. Next step (b) is rescaling, meaning that the length is shrinked so that it recovers the original lattice spacing. Name this rescaling parameter, b. In the last step (c), one makes sure that the higher level properties are the same as in the original system by readjusting the interaction parameters (Batterman 2010, p.1043), (Mainwood 2006, p.154).

In general, each transformation (or iteration) reduces or eliminates microscopic details of the system that are irrelevant for the behaviour at critical points. The result of an infinite sequence of transformations of a Hamiltonian initially at the critical point ends at a fixed point, which is the same for different systems, i.e., systems belonging to the same universal class. At the critical point, the correlation length remains infinite, where τ is the renormalization transformation. The fixed point is determined by the Hamiltonians that meet the requirement specified by equation:

$$\tau(H^*) = H^* \tag{3.20}$$

Remember that this is only true at criticality (Batterman 2010, p.1045). Notice that it is for the same reason, namely that no specific length is associated with the system at the critical point, that allows for this kind of analysis. If one looks at the model at the critical temperature one will observe clusters of all sizes of correlated atoms. The same kind of picture is repeated at different length scales. This behaviour may be identified as some sort of scale invariance meaning that the system, informally speaking, looks the same at different length scales. Because of this scale invariance, each iteration produces a new system being statistically identical to the former.

Finally, notice also the necessity of the thermodynamic limit for the divergence of the correlation length. If the lattice or block system is of finite size, then the correlation length will be limited by this size, and hence it cannot diverge (Callender and Menon 2013, p.196-197).

3.5 Summary

This chapter introduced the theory of phase transitions as the topic is treated by thermodynamics, statistical mechanics and the renormalization group. In particular, the focus has been on what was named "the problem of phase transitions"

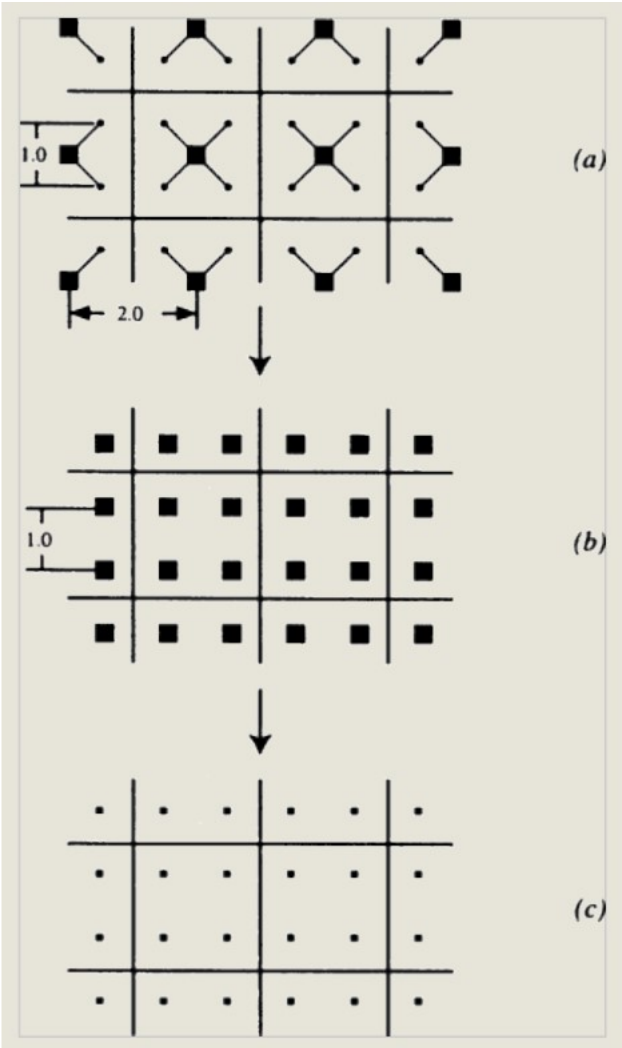


Figure 3.5: The three steps of the renormalization group real-space method. The figure is retrieved from (Batterman 2002, p.41).

and its corresponding solution. In short, the problem is that phase transitions, as they are defined in thermodynamics, cannot be directly derived from the underlying, microscopic theory, statistical mechanics. This has to do with the fact that the discontinuity required in the free energy (in either its first or second order derivative corresponding to a first and second order phase transition, respectively) by Definition 1 is mathematically impossible in finite size statistical mechanics. One closer examination, however, one observes that a discontinuity *could* occur if the system under consideration is infinite, that is, if the thermodynamic limit is implemented. Second order phase transitions, which are more commonly refereed to as critical phase transitions or critical phenomena, are identified by the system exhibiting so-called critical behaviour at the critical point (in the phase diagram). The critical behaviour (e.g. the critical exponents) is common for diverse systems that belong to the same universality class leading to the term universal phenomena or just universality. The thermodynamic limit is necessary for predicting the specific feature of universality as well.

In order to predict the behaviour close to the critical point, the tools of the renormalization group is required as the older approach to statistical mechanics, mean field theory, fails here. The renormalization method demonstrates that some microscopic details are irrelevant for the macroscopic, critical behavior. The next chapter will elaborate in which possible ways the theory described in this chapter connects to emergence.

Chapter 4

Overview: Emergence and Phase Transitions

Over approximately the last twenty years, the subject of phase transitions has gained a significantly larger role in the philosophical literature, and among this, arguments for (or against) that the topic provides evidence for emergence. There is however not only one unique way in which phase transitions are claimed to fulfil this role and the term emergence is not necessarily used in a consistent way among them either. The primary aim of the present chapter is to motivate for the possibility that phase transitions *could* be characterized by this term by looking at the arguments used for this purpose. While there certainly are alternative ways to do this, as other perspectives may exist, I have grouped the motivations or approaches into three separate main sections claiming them to represent some relevant differences with respect to this topic:

1. **The Definition of Phase Transitions and the Role of the Thermodynamic Limit**
2. **Qualitatively Different Physical Properties**
3. **Universality and the Independence of Microscopic Details**

They will all be reviewed in turn, but as the reader will observe, the first section is definitively much more comprehensive compared to the other two. This section deals with the currently theoretical treatment of phase transitions and the involvement of the thermodynamic limit. Regarding the total amount of literature about phase transitions in the context of emergence, this topic corresponds to the one most discussed. This section provides an overview of some of the main points relevant in the debate. The argument presented in the second section maintains that the physical aspects involved in phase transitions result in emergent properties in some different ways. The specific theoretical frameworks used in describing them are not involved in the claim for emergence to the same extent as the former, which makes this view contributing with some new (or different) aspects. A more recent view is presented in the third section of this chapter. There an argument for that universality, the specific feature of second order phase transitions, represents emergence is outlined. This argument is strongly related to the theoretical treatment of phase transitions offered by the renormalization group in particular but not to the specific problems that the implementation of the thermodynamic limit potentially entails for this type of explanation.

When reading this chapter, one will certainly recognise some of the characteristics used to define emergence in chapter (2), but whether or not any of the approaches and arguments listed below actually fit into the description of emergence given in that chapter will first be clarified in the next chapter where the problem formulation is answered.

4.1 The Definition of Phase Transitions and the Role of the Thermodynamic Limit

In the previous chapter the so-called "problem of phase transitions" was outlined. In short, it refers to the incapability of deriving Definition 1 (in thermodynamics) from finite size statistical mechanics. It turns out that the apparently need for the thermodynamic limit, e.i., the infinite system, in relating statistical mechanics to thermodynamics plays a crucial role in some of the arguments for that phase transitions are emergent entities. This section intends to cover different interpretations surrounding this topic and is structured as follows: First, two possible ways of formulating an argument for emergence caused by (or strongly related to) "the problem of phase transitions" are presented. Then, different ways of either supporting or avoiding this conclusion are outlined. This includes the interpretation of the thermodynamic limit as idealization in section (4.1.2). Furthermore, in section (4.1.3), the ontological or physical status of the mathematical singularity that is claimed to represent a phase transition is investigated from a critical point of view. Finally there is a section in which some of these topics are further illuminated by the actual research of phase transitions in physics today.

Recall that the thermodynamic limit is involved in the statistical mechanical treatment of phase transitions including both first and second order phase transitions, and universality. Therefore, there might be reasons to expect that its application to these different types or aspects of phase transitions could introduce some distinctive issues. However, in this section, topics of general relevance are mainly addressed. Potential issues only relevant for second order phase transitions are only barely outlined.

4.1.1 The Argument For Emergence

Below, the two ways of formulating an argument for that phase transitions are emergent, are presented. Notice that all the topics of of this section, section (4.1), are more or less concerned with them.

Liu's Formulation of the Argument

In *Explaining the Emergence of Cooperative Phenomena* (1999) Liu argues that "phase transitions are truly emergent properties." (Liu 1999, p.92). His argument is based on the fact that phase transitions, phenomena which are well-defined in thermodynamics, are mathematical impossible in statistical mechanics. Phase transitions are therefore not reducible to statistical mechanics. However, phase transitions in statistical mechanics become possible in the thermodynamic limit, but as far as we know, in reality they occur in finite systems (Liu 1999, p.93). In short: Phase transitions are emergent because they are properties of finite systems, but reducible to micro-properties of infinite systems only (Liu 1999, p.104).

Callender's Formulation of the Argument

An alternative (and more unpacked) way of presenting this argument is found in Callender (2001). Consider the four proposals below, stating facts about phase transitions as we know them:

1. real systems have finite N;
2. real systems display phase transitions;
3. phase transitions occur when the partition function has a singularity;
4. phase transitions are governed/described by classical or quantum statistical mechanics (through Z).

Then observe that, with respect to the knowledge of phase transitions presented in chapter (3), the joint of these four must be false. To avoid this conclusion one has to deny at least one of them. Those who would classify phase transitions as emergent entities will, according to Callender, reject that phase transitions are governed by statistical mechanics (proposal 4) due to the fact that there is no way to derive them within this theory restricted to finite number particle systems (which is similar to Liu's argument above). On the other hand, many physicist probably disagree with this by stating that the thermodynamic limit, at least from a pragmatic point of view, is a good approximation to a large but finite system of particles (Callender 2001, p.549-550) (This point or way of thinking will be treated in greater details below).

Callender opposes to the emergentist's conclusion above and disagrees with Liu that the failure of statistical mechanics in predicting phase transitions necessarily leads to emergence. This point is outlined in section (4.1.3).

4.1.2 The Thermodynamic Limit as Idealization

As Liu and Callender both point out, despite the fact that phase transitions are unpredictable from and irreducible to statistical mechanics, they can be predicted by the theory if one allows for that finite systems can be idealized as infinite systems. The way in which the use of thermodynamic limit is interpreted tends to affect the conclusion about whether phase transitions really represents a clear case for emergence or not. This is connected to whether or to which extent it is possible to accept or justify infinite systems in the description of phase transitions in statistical mechanics. The following sub-sections outline this aspect in terms of different points of view on the topic.

Idealization and Approximation

Firstly, a short section about idealizations and approximations in physics serves as a preface to the present topic. The phase transitions we observe and hence the phenomena to be described by theory clearly occur in finite systems as our world is restricted to such systems. Hence, the thermodynamic limit is an idealization of a real, but finite system. To this fact one can add that the thermodynamic limit is by no means the only idealization involved in physical theories. Physicists (among others) are using them all the time. But even though this is true, if one accepts the implementation of this limit in statistical mechanics, one needs a way it can be justified. That is, how can one argue that an infinite model can represent a finite, real system, in some "legitimate" way? We need to be able to show that the behaviour of a large, but still finite system approximates (in some sense) the behaviour appearing in the thermodynamic limit.[1] The sections that follow present some approaches or ways to understand this problem or more specifically the question about whether or not the thermodynamic limit as idealization is also a good approximation of the actual system.

To begin with, consider another idealization in physics applying the concept of infinity. In the article cited above, Liu compares the idealization of the infinite limit to that of regarding a rigid body in mechanics or a fluid in hydrodynamics as a differential system (Liu 1999, p.101). This is also known as the idealization of an almost continuous body (Mainwood 2006, p.230). I will review Liu's short description of this idealization here (see Liu 1999, p.101-102). Consider the following equation representing the density of a solid in the limit $\Delta V \to 0$:

$$\rho_M = \lim_{\Delta V \to 0} \frac{\Delta M}{\Delta V} = \frac{dM}{dV} \tag{4.1}$$

The question is whether $\frac{dM}{dV}$ is a good[2] approximation of the actual mass density, $\frac{\Delta M}{\Delta V}$ or not, or in other words if on the way to the limit $\Delta V \to 0$, $\frac{\Delta M}{\Delta V}$ approaches $\frac{dM}{dV}$. We can think of a set of $\left(\frac{\Delta M}{\Delta V}\right)_n$ where ΔV_n gets smaller and smaller for each n (as $n \to \infty$). It can be shown that $\frac{\Delta M}{\Delta V} \approx \frac{dM}{dV}$ when ΔV_n is (very) small.[3]

[1] Ideally, the topic of idealizations and approximations in physics should have been treated much more carefully than what it is here. One could for instance distinguish between idealizations that, even though not present in the actual case, still are possible in the real world, and those that actually are impossible. But as the topic in this thesis is emergence in particular I have considered to restrict the amount of information to what I find directly relevant to this, which I think is sufficient to make the point I want to make.

[2] What is meant by "good" may of course raise new questions. But in this context, it often means something like cases where big, finite systems smoothly approach the behaviour at the infinite limit.

[3] This is not a mathematical proof (see Liu 1999, p.101).

Liu concludes that in this case, an actual solid which is densely packed with small molecules does not differ that much from the idealized case in the limit, and hence this limit may serve as a good approximation of the actual solid. In this sense one can rightly represent the actual solid by so-called limit quantities (such as ρ_∞) (Liu 1999, p.101). So, if this argument holds, can the use of the thermodynamic limit for the purpose of identifying phase transitions be justified as well?

The Limit Is Not Justified

In addition to the the argument that phase transitions are emergent properties outlined above, Liu investigates the nature of thermodynamic limit and whether or not it could serve as a good approximation for a real, but finite system. Immediately, one could state that infinity is at least for practical purposes indistinguishable from a system consisting of order of magnitude 10^{23} number of particles. While Liu does not oppose to the use of idealizations and approximate methods in physics in general (as pinpointed above), he rejects that the thermodynamic limit can be justified in the same way as in the case of the density of a solid above (Liu 1999, p.101). In principle one could have defined limit quantities (at infinity) to represent the thermodynamic quantities, as done in the mass density example, but the conclusion made there does not seem to generalize to the case of phase transitions even though the two examples might look similar. Liu defends his view by stating that:

> "*(i) at no stage of the process in which $V, N \to \infty$ is a singularity of a system even roughly or approximately defined, (ii) nor is the singularity approached or approximated in any proper sense of approach or approximation.*" (Liu 1999, p.102).

Liu claims that the thermodynamic limit has nothing to do with approximation. This is because the required singularity is not approximately defined on the way to the limit ($N \to \infty$). In order to understand this recall the solution given by Lee and Yang in section (3.3.2) and particularly Theorem 3: It was shown that only at the intersection between the unit circle and the real x-axis, $z = 1$, a physically meaningful root can be found (which is required for the singularity to be obtained and only possible at $N = \infty$). Therefore, no other value, even though extremely close to 1, can approximate a phase transition, in either the two dimensional Ising model of a ferromagnet or a lattice gas (Liu 1999, p.101-102).

While there are beneficial reasons for applying the thermodynamic limit, we have no explanation for why it can be used in the first place (due to the disagreement between the infinite system and the finite system), and hence it cannot be justified (Liu 1999, p.102).

Justifying the Limit - A Mathematical Analogy

In contrast to the view above, Butterfield (2010) argues that the behaviour at the thermodynamic limit can be approximated by the behaviour of a large, finite system. In *Less is Different: Emergence and Reduction Reconciled* (2010), he presents a mathematical analogy which aims to resolve what he describes as a misunderstood "mystery" of phase transitions. By this he claims to show that large finite systems actually approach the hypothetical behaviour of an infinite system (Butterfield 2010, p.1077). The following is a review of Butterfield's analogy. It is based on Butterfield's formulation of the analogy (see Butterfield 2010, p.1077-1082) with assistants from a slightly simpler version provided in (Callender and Menon 2013, p.212-214), in which the authors seem to agree with Butterfield's view on this point.

The idea is to think of two sequences of real functions, $g(x)_N$ and $f(x)_N$, where $N \in \mathbb{N}$. First, consider the former of these two:

$$g(x)_N = \begin{cases} -1 \quad \text{for} \quad x \leq \frac{-1}{N} \\ \\ Nx \quad \text{for} \quad \frac{-1}{N} < x < \frac{1}{N} \\ \\ 1 \quad \text{for} \quad x \geq \frac{1}{N} \end{cases} \tag{4.2}$$

Regarding how $g(x)_N$ is defined one observes that for all finite values of N, the function $g(x)_N$ is continuous and that $g(0)_N = 0$. The slope, connecting the two constant functions, in the range $x \in \{\frac{-1}{N}, \frac{1}{N}\}$ gets steeper and steeper as N increases. At $N = \infty$, $g(x)_N$ will be discontinuous at $x = 0$, and we may name this function $g(x)_\infty$.

Then, the other function, $f(x)_N$, is defined with respect to $g(x)_N$ by:

$$f(x)_N = \begin{cases} 0 \quad \text{if} \quad g(x)_N \quad \text{continuous at x} \\ \\ 1 \quad \text{if} \quad g(x)_N \quad \text{discontinuous at x} \end{cases} \tag{4.3}$$

$f(x)_N$ is a two valued function. It is a constant function equal to zero for all finite N. But $f(0)_\infty = 1$, so $f(x)_\infty$ becomes discontinuous. If one focuses on $f(x)_N$ alone, forgetting about its connection to $g(x)_N$,[4] the discontinuity may look mysterious, in the way that the behaviour at $x = 0$ in the infinite case seems incomparable to the finite N cases regardless of how large value N might take.

According to Butterfield, the case above translates directly to the case of phase transitions: One may think of the phenomenon of phase transitions as being represented by the value 1 by the mathematical model $f(x)_N$ and N representing the number of particles. Hence, the property is only modelled by the infinite case, as $f(x)_N = 1$ only for $N = \infty$ by what happens at $x = 0$. To explain this behaviour, or to argue that it make sense to model phase transitions as such seems to be unjustified due to the apparent disagreement with the finite N cases. But this is just the case when paying attention to $f(x)_N$ alone. Because, if we rather focus on $g(x)_N$ and $g(x)_\infty$ and how the former approaches the latter as N increases, we observe that the difference between the two becomes arbitrarily small. The slope or the gradient of $g(x)_N$ approximates very well $g(x)_\infty$ for large N, but the same is much harder to see in the case of $f(x)_\infty$ and $f(x)_N$ (Butterfield 2010, p.1079).

[4]Doing this may look like and unsolvable task, as $f(x)_N$ actually *is* inextricably linked to $g(x)_N$. So to think of $f(x)_N$ without thinking about how it is generated by $g(x)_N$ must mean, I would propose, the task of visualizing the graph drawn by $f(x)_N$ directly.

So the main point of the mathematical analogy just reproduced was to suggest a way of "demystifying" the behaviour at infinite N compared to that of finite N's, meaning that the behaviour at the limit can be approximated by the behaviour before the limit. Nevertheless, Butterfield still thinks that phase transitions serves as an example of emergence is physics. Emergence is, according to Butterfield, "behaviour that is novel and robust relative to some comparison class." (Butterfield 2010, p.1066). One example of a comparison class is *limits* (taking some crucial value, for instance 0 or ∞) so that the novel and robust behaviour occurs in this limit compared to the behaviour of, in this case, a finite system. In Butterfield's view emergence can, but need not imply a failure of reduction. That emergence can be compatible with reduction is exemplified by exactly phase transitions, since taking the thermodynamic limit allows us to deduce emergent behavior (as he defines it). According to Butterfield there are two kinds of emergence involved in the case of phase transitions: Strong and weak emergence. Butterfield does not claim the thermodynamic limit to represent anything "physically real" (a topic to be investigated in greater details in section (4.1.3) below). What is physically real happens before that limit, meaning that we can understand this "novel and robust behaviour", the phase transition, in the case of a large finite system, as the analogy above illustrated. These two, the behaviour at the limit and the behaviour before the limit, are called respectively strong and weak senses of emergence being compatible with the idea of reduction (Butterfield 2010, p.1066-1071).

In Callender and Menon (2013) the authors argue in a similar way that a large system can approximate the behaviour appearing in the infinite idealization (this is done with the aid of the same mathematical analogy):

> "*To see the connection between a phase transition defined via Def 1 and real finite systems, one must first "undo" the conceptual innovation and write the theory as a limit of nascent functions. At that point one can then see that the idealization is an innocent simplification and extrapolation of what happens to certain physical curves when N grows large.*" (Callender and Menon 2013, p.214).[5]

Therefore, they conclude that phase transitions *are* explanatory reducible to statistical mechanics and hence no strong argument for emergence follows from the apparently need for the infinite idealization (Callender and Menon 2013, p.222). Notice that Butterfield in contrast argues that phase transitions represent emergent behaviour even if the use of the limit can be justified. This connects to that he is defending the view that emergence and reduction are compatible ideas. A rather different argument for why the use of limit should be accepted is found in Batterman (2005).

Justifying the Limit - Necessary Singularities

In the article *Critical phenomena and breaking drops: Infinite idealizations in physics* (2005) Batterman generally defends the view that the infinite idealization is abso-

[5]What is named Def 1 corresponds to Definition 1 in this thesis.

lutely essential in the statistical mechanical explanation of phase transitions and hence it cannot be replaced by any other approaches. Even though real systems are finite, we cannot understand them without the infinite idealization (Batterman 2005, p.231). Batterman never directly uses the term emergence in this article, but the points argued for are nevertheless making a basis for at least some interesting aspects of phase transitions and emergence (see below). However, in Batterman (2010) it is stated explicitly that the qualitative change in state we observe in phase transitions and critical phenomena "... are indeed emergent phenomena." (Batterman 2010, p.1033). His argument is that these qualitatively changes are genuinely novel because they require the infinite idealization and the fundamental theory, statistical mechanics, dealing only with a finite number of particles, becomes insufficient (Batterman 2010, p.1033-1034). This argument is in some ways akin to the two arguments section (4.1.1.). What makes Batterman's argument different from e.g., Liu's argument is that he thinks that the limit is justified.

Batterman (2005) argues in particular that it is the failure of reductive relations between thermodynamics and statistical mechanics at critical points and phase transitions that justifies the infinite idealization (Batterman 2005, p.227). This has to do with to what he names *singular limits*, which only tends to appear at critical points (and not at phase transitions in general).[6] Therefore, it might be that the point made here only applies to second order phase transitions. I will not go further with the notion of singular limits and the possible consequence it has for separating between first order phase transitions and second order phase transitions, but rather refer the reader to the original paper[7] as the reasons Batterman gives for this distinction is not exactly what I am looking for here. A more interesting (or relevant point) for the purposes of this thesis is Batterman's interpretation of the singularity that represents the phase transition, see section (4.1.3) just below this one.

Before changing to that topic, some final comments about the role of the thermodynamic limit involved in the explanation of the particular feature of universal behaviour at critical points is offered. Recall that universality is not recognized at first order transitions. The universal behaviour of classes of (different microscopical) systems at their respective critical points has resulted in (at least) two different motivations for emergence and the first of these will be presented in the following as it has to do with the need for the thermodynamic limit, in order to predict or explain this common behaviour from the underlying theory. The second motivation is postponed to section (4.3). The explanation for universality, provided by the renormalization group, depends upon infinities and divergences. They are referred to as *necessary* singularities (Batterman 2010, p.1040). Statistical mechanics is incapable of capturing the macroscopic behaviour of universality (Batterman 2010, p.1033-1034). Batterman's recurring point is that these infinities and divergences are absolutely essential for this explanation: the explanation of the universality of critical phenomena and the "flow" to the fixed point. In this context, it is the correlation length that needs to diverge which can only happen in the termodynamic

[6] The term 'singular' here should not be confused with the singularity in the thermodynamic potential in both kinds of phase transitions.

[7] See Batterman (2005) for details of his explanation.

limit (Batterman 2010, p.1037, 1047), see also section (3.4). Hence, Batterman does not seem to allow for that any finite size system can approximate this behaviour (see Batterman 2010, p.1047-1049). It is not just that singularities are essential for explaining universality in this view. Batterman also suggests that there is no reason to avoid them and think of them as unphysical or unreasonable. Rather they should be interpreted as sources of information about the world (Batterman 2010, p.1049).

4.1.3 The Singularity as Model or Reality

The different perspectives or interpretations of the thermodynamic limit as idealization presented above disagree to some extent about the question of whether or not (or in which way) the limit can be justified in the case of phase transitions. Another issue that could affect the way we evaluate whether phase transitions are emergent entities or not is connected to the potential difference between phase transitions in nature and phase transitions as they are defined by Definition 1, as discontinuities in the thermodynamic potential. Should the definition in thermodynamics be interpreted literally?

Phase Transitions Are Real Singularities

The question about the "realness" of the mathematical representation of phase transitions is addressed in Batterman (2005). Batterman distinguishes between so-called *physical discontinuities* and *mathematical discontinues*. The observed qualitative distinction between different phases in a fluid or between the phases of a magnet above and below the critical point exemplify physical discontinuities. These are therefore naturally represented mathematically as they are by Definition 1. One might bring into question if these representations are in fact real physical discontinuities. Batterman's answer is yes. First he takes a more careful position stating that: "It is true that we do not see the topological change in the phase transition (say when we witness water boiling in a tea kettle) [...] But that, by itself, does not show that there is no genuine physical discontinuity in the thermodynamic system." (Batterman 2005, p.234). He continues by stating that if one does not believe in the existence of physical discontinuities, then there is no reason for statistical mechanics to employ the thermodynamic limit either. But if there *are* physical discontinuities, which is the position he supports, then the limit is absolutely necessary for statistical mechanics to be able to even establish that distinct phases of systems exist. (Batterman 2005, p.234). Notice that this points seems to apply to all kinds of phase transitions.

Phase Transitions Are Not Real Singularities

Batterman's proposal about that phase transitions are physical (or real) discontinuities is among others challenged in Callender and Menon (2013). While distinct phases may appear as macroscopically and qualitatively distinct to us we have no guarantee that the transition is in fact a singularity. They state that it even might be misleading to describe the transition as causing a qualitative change, because: "...from a thermodynamic perspective the difference is quantitative. Phases are distinguished based on the magnitudes of certain thermodynamic parameters." (Callender and Menon 2013, p.215).

Callender (2001) also argues against that the singularity is real. As a response to the way in which emergentists could argue for the emergence of phase transitions as outlined in his argument in section (4.1.1), Callender suggests that we should rather considering the denial of proposal 3, which is according to him the weakest of the four proposals (Callender 2001, p.550). Recall the content of Callender's proposal 3: phase transitions occur when the partition function has a singularity. He argues that phase transitions, among several other familiar examples,[8] are sometimes thought of as representing emergent phenomena, but that this is so because we are taking the concepts defined in classical thermodynamics too seriously or too literally. And this comes to affect how we interpret or understand the relationship between this theory and the so called underlying microscopic theory, statistical mechanics (Callender 2001, p.540-542). Additionally, Callender argues, that the fact that phase transitions are defined as mathematical singularities in thermodynamics does not forces us to treat them as such in statistical mechanics as well, even though there are good pragmatic reasons for thinking of the phenomenon as a singularity in the partition function. This is a part of what seems to be his general view relating to questions about relationships between theories: we cannot necessarily require the mathematical definitions to be exactly the same across levels (Callender 2001, p.550).

A point somehow similar to Callender's point above is also Liu's final conclusion. Despite his conclusion supporting that phase transitions represent emergent properties, he suggests that one should hope for a conceptual shift in thermodynamics meaning a shift in the way in which phase transitions are defined. Phase transitions are defined as they are in thermodynamics (as singularities), due to that thermodynamic systems are idealized as continuous matter. Hence there are no fluctuations[9] in such systems. To reproduce the singularity in statistical mechanics the infinite idealization is required (the fluctuations disappear here). So the two theories are both idealized but in separate ways. The idealization of thermodynamic systems as dense is justified while the idealization of statistical mechanics as describing infinite systems is not (see the former sections upon this). But we know that there are fluctuations in real thermodynamic systems. Therefore the representation of phase transitions as singularities in this theory is an artifact and it is this artifact that forces statistical mechanics to make use of the thermodynamic limit. Hence the job done by the thermodynamic limit is not to save the phenomenon of phase transitions, as phase transitions appearing in finite systems (with fluctuations), cannot be real singularities. What the thermodynamic limit does for it, is to save the theory (thermodynamics) stating that a phase transition is a singularity, not the

[8]E.g., the second law of thermodynamics and the concept of equilibrium.

[9]These thermal fluctuations should that disappear in the thermodynamic limit should not be confused with the fluctuations that dominate near the critical point associated with the divergence of the correlation length.

phenomenon it self (Liu 1999, p.102-105).

Callender and Liu agree to that phase transitions in real systems cannot be real singularities. In the real world, there are thermal fluctuations and hence, what we measure cannot be perfect singularities either (Callender 2001, p. 550). The difference between the two views can be seen by how the term emergence is related to this. According to Liu, the insufficiency of statistical mechanics leads to the claim about emergence, while Callender, as described above, throws doubts on whether it is really necessary that theories across levels (such as thermodynamics and statistical mechanics) must represent a phenomenon in exactly the same way.

4.1.4 Perspective: Phase Transitions in Theory and Experiment

So far this section has focused on the definition of phase transitions and the conceptual issues involved in applying the thermodynamic limit in statistical mechanics. Some arguments against that Definition 1 (or thermodynamics) correctly describe phase transitions have already been presented (e.g., Liu (1999) and Callender (2001)). This final subsection moreover looks at phase transitions as they are studied by an empirical science and the possibility that such aspects also could affect how the case for emergence in this context should be evaluated. Seen from the point of view of a physicist,[10] the following (additional) perspectives are often taken into account as well.

The Benefits of the Limit

In the previous sections we have seen that there are theoretical benefits of employing the thermodynamic limit in statistical mechanics. Examples hereof are its involvement the Lee and Yang theory and the renormalization group. Almost all the successful treatments of phase transitions within statistical mechanics apply the thermodynamic limit (Mainwood 2006, p.213). Beyond the theoretical or mathematical success of the infinite limit, is however its empirical success, meaning the agreement with experimental results. In real experiments, the systems contain a large number of particles which are, compared to particle dimensions, located in large volumes. But none of N or V are exactly infinite as they are in the thermodynamic limit. Even though this is true, phase transitions observed as apparently singularities occur in these systems. The point is that in many cases these so-called observed singularities agree with the theoretical predictions caused by calculations where the thermodynamic limit is involved. The agreement between the theory of an infinite system and phase transitions in observed finite systems could be due to that so-called finite-size effects often are outside experimental resolution or at least the difficulty of separating these effects from other effects due to gravity or impurities (Barber 1983, p.146-147).

[10]This is not to claim that all physicists treat the matter as such nor that it less interesting for the philosophical analysis.

The Limits of the Limit and the Search for Alternative Definitions

Despite the benefits of the thermodynamic limit for theoretical purposes as well as these results coincides with at least some experimental results, the way we understand phase transitions is still an on-going research area in physics (Butterfield 2010, p. 1124), (Callender and Menon 2013, p.206). There are at least two reasons for why it could be worth considering other possibilities to the currently theoretical treatment of phase transitions: One is the hope for avoiding taking the thermodynamic limit, that is, developing a theory of phase transitions which applies to finite systems in the first place. These are often referred to as *smooth phase transitions* (Callender and Menon 2013, p.206). The other is that Definition 1 tends to be insufficient in capturing all possible kinds of phase transitions that might exist for different physical systems. By this I mean the problem that there are systems apparently exhibiting phase transitions, which are excluded by lacking a well-defined thermodynamic limit. To concretize this point, recall the particle system defined by Lee and Yang in section (3.3.2). Even though the conditions that determine these systems are quite general, the assumption made about the range of the forces between the particles clearly shuts out long-range forces systems. This is important because such systems, among others, also suffer abrupt macroscopic changes which could in principle be incorporated in the concept we name phase transitions (Callender and Menon 2013, p.205), (Butterfield 2010, p.1072). Another example is the transition from metal to insulator, where one does not know whether the transition is of first or second order so that it is not obvious how to classify this phenomenon within the existing framework (Kadanoff 2000, p.213).

The fact that several systems, apparently exhibiting phase transitions, do not fit in to the current theoretical framework and specifically that some of these systems lack a well-defined thermodynamic limit might raise some questions: Is definition 1, if correct at all, sufficient for the task of modelling the phenomenon of phase transitions? Do we search for another, more inclusive definition of phase transitions in the future? Could it even be the case that the concept of phase transitions must be thought of as a cluster concept meaning that different systems claim different definitions to correctly describe the phase transition they undergo? Can some systems be studied as infinite and others as finite? Callender and Menon suggest that:

> "*We believe, to the contrary, that no theory, infinite or finite, statistical mechanical or mechanical, possesses a natural kind that perfectly overlaps with the thermodynamic natural kind.*" (Callender and Menon 2013, p.205)

As a result of these considerations, one might conclude that the very focus on Definition 1 and the thermodynamic limit leads to an investigation of phase transitions of limited scope and relevance.

4.2 Qualitatively Different Physical Properties

The previous section focused on the thermodynamic definition of phase transitions and whether or not statistical mechanics as a fundamental theory is sufficient to explain them. This section presents an approach to phase transitions and emergence in which this definition and the use of the thermodynamic limit do not play the crucial role. Alternatively, when setting the specific theoretical details aside one can focus more directly on the physical aspects associated with phase transitions in stead i.e. the properties and processes involved.[11] At the very phenomenological or observable level, we often identify phase transitions with abrupt changes in the state of matter. Similarly, one can think of going trough a phase transition, e.g., from liquid water to an ice cube, as a qualitative change in behaviour of that material. This statement does not contribute with anything new or controversial as it clearly matches the macroscopic and qualitative descriptions we use about phase transitions, a recurring point in this thesis. The apparently qualitative change in behaviour is of course also the primary reason for the theoretical description, i.e., the discontinuity. What it adds to this chapter is a new way in which emergence is used in the context of phase transitions which is more intuitive or less technical. In the section below a perspective that could fit into the description just given is elaborated.

4.2.1 Liquidity and Ferromagnetism as Emergent Properties

In *Emergence: A Philosophical Account* (2016), Humphreys argues that first order phase transitions in fluids and the second order phase transition from paramagnetism to ferromagnetism both result in emergent behaviour and that this behaviour exemplifies diachronic, ontological emergence. While these examples apparently are the same as those already applied in this thesis Humphreys's account of emergence in these cases, generally highlights the physical aspects and interactions giving rise to phase transitions and the properties resulting from them in a more direct way. Mathematical and more abstract aspects are omitted. Humphreys defines emergence in terms of a list of four features: "Emergent features result from something else, they possess a certain kind of novelty with respect to the features from which they develop, they are autonomous from the features from which they develop, and they exhibit a form of holism." (Humphreys 2016, p.26). One or several of them must be recognized in the particular case in order to claim emergence.[12]

[11] This is not to say that the perspectives introduced in section (4.1) are not about physical systems. However, the points outlined there are intimately connected to the specific definitions and theoretical tools involved in the explanation of phase transitions today.

[12] Notice that emergence is defined in a way comparable to Kim's doctrines of emergence in chapter (2). In this context it should be noted that I have simplified Humphreys' allover view on emergence as the examples about phase transitions are retrieved from an rich book on the topic of emergence in philosophy and science. The aspects to be outlined here do of course not cover the total content as the book presents and supports varies ways of being emergent. In this way, Humphreys treats the term 'emergence' more generally and more carefully than those views referred to in the the former sections as the articles they belong to are concerned with phase

To see in which possible ways his account of emergence of phase transitions work (and differs from other accounts) consider the two examples just mentioned. Common for both these kinds of transitions is that the beginning and end of the process involve qualitative different properties. This feature is important in order to establish the claim about ontological emergence (Humphreys 2016, p.252). The emergent behaviour is due to the new physical properties that appear after the relevant transition has occurred. The transition from a solid crystal to its liquid phase, for instance, is a physical process from order to disorder in which the property of the liquid emerges from the qualitatively different property of the solid. The emergent properties involved in a transition from solid to liquid (or the other way around) are therefore either liquidity or rigidity, respectively. Notice that in Humphreys' view it is not the phase transition that is the emergent entity. Rather it is a new phase (defined in terms of properties) that *emerges* from another qualitatively distinct phase. Humphreys claims all the four features to be present in the case of an ordered state emerges from an disordered state: First it is a state resulting from another state. Second (and third) the state after the transition has occurred is both novel and autonomous compared to the original state. Finally, the property, liquidity, is by it self holistic (Humphreys 2016, p.47).[13] The latter example, ferromagnetism is examined more deeply. Here Humphreys offers a more detailed description of the magnetic system comparable to the one of the fluid system given in section (3.2.2). As I have not provided the same theoretical foundation of the ferromagnetic case, I will not review all the details here. Anyway it is still the real physical property of ferromagnetism that is the emergent property. For the same reason as in the solid-to-liquid example, ferromagnetism is an emergent property as it is an ordered state arising from and disordered state as a result of spontaneous symmetry breaking (Humphreys 2016, p.255).

Humphreys addresses that there could be a difference between emergence occurring in models and emergence occurring in natural systems (see Humphreys 2016, p.8). Identifying cases as ontological emergence requires that one allows the model we use when describing them to accurately describe the real systems they are meant to model (Humphreys 2016, p.45, 256).

transitions alone.

[13]The holistic feature is a property of a macroscopic system in general. It is an emergent property due to that it "cannot be possessed by individuals at the lower level because they occur only in the case of infinite collections of constituents." (Humphreys 2016, p.252). However, while Humphreys is completely aware of the issues raised by the infinite systems and also that others have emphasized these issues in the context of emergence (see Humphreys 2016, p.256 - 258), he is not particularly discussing the difference between an enormous finite collection of particles and an infinite as was one of the main topics in section (4.1). Rather Humphreys tends to defend a view about the use of the thermodynamic limit being similar with some of the more pragmatic views presented in section (4.1): A macroscopic system is identified as one whose equation of state is independent of size (meaning that the thermodynamic limit is applied). The real macroscopic systems are those being sufficiently large so that they cannot be empirically distinguished from the ideal macroscopic systems (Humphreys 2016, p.249-250).

4.3 Universality and the Independence of Microscopic Details

The final section of this chapter presents a view of emergence which is only about the specific feature at critical points, universal behaviour. The argument to be outlined below is based on the fact that systems belonging to the same universal class (described by different Hamiltonians) exhibit (some of) the same macroscopic behaviour at their respective critical points. In other words, the universal behaviour at criticality exhibited by different systems shows that the microscopical details distinguishing these systems from one another are irrelevant for the explanation of this behaviour (provided by the renormaization group). There is a kind of independence between the microscopic and the macroscopic level with respect to this behavior. This view is more specifically developed and defended in Morrison (2015) and a similar view is also supported in Batterman (2002, 2010), see below.

Their views upon universality are inspired by or share some of the ideas about emergence suggested in *The Theory of Everything* (2008) by Laughlin and Pines,[14] a second influential paper to be incorporated in the somehow same "tradition" as Anderson's *More is Different* (2008), mentioned in the introduction chapter. Here the authors suggest a term "protectorates", being either quantum or classical which they refer to as: "a stable state of matter whose generic low-energy properties are determined by a higher organizing principle and nothing else." (Laughlin and Pines 2008, p.261). Furthermore: "The emergent physical phenomena regulated by higher organizing principles have a property, namely their insensitivity to microscopics." (Laughlin and Pines 2008, p.261) It is claimed that these so-called "higher organizational principle" cannot be obtained from anything like a "theory of everything". (Laughlin and Pines 2008, p.260). They take spontaneous symmetry breaking, involved in phase transitions, to exemplify such a principle (Laughlin and Pines 2008, p.261).

4.3.1 Stable Macroscopic Behaviour

In *Why Is More Different* (2015), Morrison emphasizes the aspects of universal behaviour as the independence or irrelevance of microscopical details of the particular system. In this article the phenomenon or theory of *superconductivity* is the primary working example to illustrate the main point about emergence. Superconductivity also involves phase transitions and critical behaviour, but the description required is more technical compared to phase transitions taking place in fluid (or magnetic) systems described in chapter (3). Anyway, her conclusion seems to generalize to the universal behaviour in other systems too.[15] About the physical phenomenon under consideration, she pinpoints that:

> "*..., it isn't that instances of superconductivity in metals don't involve*

[14]First published in 1999.

[15]Notice that superconductivity does not correspond to the same universal class as fluids and magnetic systems.

micro-processes, rather the characteristics that define the superconducting state are not explained or predicted from those processes and are independent of them in the sense that changes to the microphysical base would not affect the emergence of (universal) superconducting properties." (Morrison 2015, p.102).

Remember that that the fact that different microscopic systems exhibit the same behaviour is by no means a pure theoretical result. It was first of all confirmed experimentally, an observation the mean field theory was incapable to explain. Today the tools of the renormalization group are claimed to provide an explanation of the universal behaviour and the specific kind of explanation this is, is important to Morrison's view on emergence in general.

Predicting and Explaining Universality - A None-Reductive Account

According to Morrsion, terms as 'surprising' and 'novel' should not be what characterize emergent phenomena (Morrison 2015, p.113). Due to the development of the renormalization group universal behaviour is both predictable and explainable, but as the renormalization group is a general framework that applies to a variety of theoretical contexts, it does not corresponds to a fundamental theory. Hence it is not a reductive explanation. What characterizes a fundamental theory is that is concerned with specific types of physical systems and emphasizes details of these systems (Morrison 2015, p.101). In contrast, the explanatory tools involved in the method of the renormalization group are general features which are independent of the microscopic physics or structure investigated. One could object to this that we cannot know that none of the properties of the smaller constituents influence the macroscopic behaviour at critical points, just because the techniques involved in the renormalization group explanation of universality ignores these details. But, Morrison argues, none of the features determining this behaviour are detail-depended. The only features relevant are such as the symmetry and dimensionality of the system (Morrison 2015, p. 112). The method of the renormalization group is essential because it demonstrates the so-called defining features for emergence, according to Morrison: Both the epistemological and the ontological independence between different energy levels. (Morrison 2015, p.107). It is not only that we need not refer to microscopic details in order to explain the macroscopic behavior at the critical points (epistemic independence). The fact that we often idealize or model systems by simplifying and ignoring details about them of less importance for the explanation of one certain level compared to another is not by itself enough to claim emergence. What makes this behaviour emergent is that we cannot appeal to the microscopic details (ontological independence). In the case of fluid and magnetic systems for instance, their similar behaviour at criticality indicates that it is independent of and immune to changes in the micro constituents even though they arise from them. To put it in another way, the fact that different systems belong to the same universal class, indicates that no new microscopic theory is able to provide a reductive explanation of universality even in the future. This emergent behaviour is stable (Morrison 2015, p.111-113). Additionally, the renormalization group method

"...reveal the nature of this ontological independence by demonstrating the features of universality and how successive transformations give you a Hamiltonian for an ensemble that contains very different couplings from those that governed the initial ensemble." (Morrison 2015, p.110).

A comparable point about emergence and universality is made in Batterman (2010). The so-called "emergent protectorates" are, according to him: "...stable states of matter that are in effect decoupled and largely independent of physics at shorter length/higher energy scales." (Batterman 2010, p.1041) The notion of "emergent protectorates", originally appearing in Pines and Laughlin (2008), refers as explained above to stable states of matter depending on higher organizational principles alone. Batterman takes their example of these principles, e.g., spontaneous symmetry breaking to be unsatisfactory alone when we have the renormalization group which also *explains why* the micro details are irrelevant. Batterman also thinks of this kind of explanation which the renormalization group exemplifies as a special kind of explanation, a point in which the philosophical literature about explanation have overlooked, and names this method of eliminating irrelevant details for *asymptotic explanation* (see Batterman 2002, p.22).

As a final comment, it should be noted that as described in section (3.4), the thermodynamic limit is involved in the renormalization group account of universality as well. Morrison agrees to that the explanation presupposing an infinite number of particles is not entirely unproblematic. But she agrees with Batterman[16] that even though we observes stable and universal behaviour in finite systems, as this behaviour is an experimental fact first of all, we cannot *understand* this behaviour without the tools of the renormalization group. The fixed point requires the limit. Hence the thermodynamic limit is essential for this explanation (Morrison 2015, p.107, 110). Notice that the thermodynamic limit is not directly involved in the argument for why universality is emergent behaviour in Morrison's argument even if she argues that it cannot be omitted.

[16]As pointed out in *Necessary Singularities* in section (4.1.2), Batterman emphasized the necessity of the thermodynamic limit. Without it, one would not be able to predict critical and universal behaviour (Batterman 2010, p.1038). Batterman concludes that it unlikely that a more fundamental theory, without singularities and divergences, will ever be able to explain the existence of these protectorates (Batterman 2010, p.1041).

Chapter 5

Discussion and Clarification

The sections (4.1-4.3) dealt with phase transitions as potentially emergent entities, but as we saw, the term emergence is not necessarily used in a consistent way among all the different ways in which phase transitions were claimed to fulfil (or not fulfil) this role. In this chapter the aim is nevertheless to discuss and clarify the case for emergence of phase transitions. I will return to emergence as it was described in chapter (2) and evaluate whether this description more specifically apply to phase transitions. The themes and issues addressed in the former chapter guide this work. Section (5.1) is directed to the first sub-question in the problem formulation while section (5.2) is directed to the second sub-question. Based on these considerations, the chapter is concluded by a final section, where the problem formulation of the thesis is answered.

5.1 Do Phase Transitions Fulfil the Role of Emergence?

Recall from chapter (2) that the two necessary conditions involved in an emergent relation is the autonomy of what is claimed to be emergent and the dependency-relation to its base. Moreover this claim can be specified by a selection of characteristics or leading ideas of emergence (Kim's doctrines of emergence):

1. Relation between Parts and Wholes
2. Unpredictability
3. Irreducibility
4. Unexplainability

In the following section I will, as far as possible, discuss and evaluate the presence or lack of each of the characteristics, with respect to the arguments for emergence presented in the sections (4.1-4.3). Additionally, an entity can be emergent in several ways. One can (for instance) distinguish between epistemological and ontological emergence or synchronic and diachronic emergence. The points to be outlined aim to answer the first part of the problem formulation:

To what extent and in which way do phase transitions fulfil the role of emergence?

I will answer this by first drawing the positive account for that phase transitions are emergent entities. Thereafter some critical aspects are addressed.

5.1.1 Definition 1 and Emergence

The definition of phase transitions in thermodynamics and the incapability of statistical mechanics as a fundamental or microscopic theory to reproduce this definition without the thermodynamic limit ("the problem of phase transitions") has led many to classify phase transitions as emergent entities.[1] At closer examination, this conclusion is however not that obvious, or at least the case is more complicated than first expected.

The Case for Emergence

The potential emergent entity in this case is thus the thermodynamic definition of phase transitions as a discontinuity in the thermodynamic potential. Consider first the characteristic describing emergence as a relationship between the whole and its parts or eventually the holistic feature of emergence. Phase transitions are in this sense higher-level entities/properties raising from a system of interacting particles. Since these higher-level properties (defined by thermodynamics) cannot be predicted from statistical mechanics, the lower-level theory claimed to describe the physics of these particles, this kind of relation between the parts and the whole is the the one required to claim emergence (compared to resultants in which the whole, even if it is a complex entity, may be predicted from the information about the interactions between its parts). The phase transition, the whole, cannot be fully reduced to its parts which also causes a failure of explanation of phase transitions (in terms of the fundamental theory, statistical mechanics).

If one accepts that phase transitions are emergent entities due to the recognition of the characteristics, one can add to the description that it is synchronic emergence rather than diachronic emergence since the property of phase transitions takes place simultaneously in the upper and the lower-level theory or description.[2]

Furthermore, regarding the distinction between epistemological and ontological emergence, the most obvious would be to think of this as epistemological emergence as two theories are involved and we do not know whether any of them are able to correctly describe real phase transitions. However, if one thinks of Definition 1 as being the real description of phase transitions, a view which seems to be coinciding with Batterman's "real singularities", one can imagine that there is a case for

[1]Recall Liu's argument for emergence: Phase transitions are emergent because they are properties of finite systems, but reducible to micro-properties of infinite systems only (Liu 1999, p.104). Or Callender's four proposals each stating apparently true statements about phase transitions, but together imply inconsistency, see section (4.1.1).

[2]It is true of course that phase transitions are processes in time but the time-aspect is not taken into account or has no relevance when discussing two levels of description of the same phenomenon.

ontological emergence as well.[3] I will elaborate this point below.

Critical Remarks

Despite what was just stated, the positive summary of why phase transitions could be regarded as emergent entities and what kind of emergent entities they are, I think that the case for emergence needs to be handled more cautiously. First, as we have both a macroscopic theory and a microscopic theory to describe the subject of phase transitions, one phenomenon and potentially two theoretical descriptions are involved: the observed phenomenon, thermodynamics and statistical mechanics. This makes the case a bit more complicated as for instance if there where only one theory available to describe the phenomenon observed. Recall that Liu states that phase transitions are emergent properties, but he expect them to be defined otherwise by a future theory. Callender additionally suggests that statistical mechanics is not necessarily forced to identify phase transitions in the same way as thermodynamics. According to Batterman, phase transitions represent a case were the so-called mathematical and physical discontinuities are expected to be the same. An additional point is however that statistical mechanics, as a statistical theory, is not obviously the most fundamental theory that could be used to describe phase transitions. Finally, the fact that many systems, apparently exhibiting phase transitions, lack a well-defined thermodynamic limit and that research with the aim of finding alternative ways of defining them is going at least suggests that the way phase transitions has been discussed here, is of limited scope. To take a stand to all the considerations mentioned above is outside the scope of this thesis, but in order to determine what kind of emergence that phase transitions eventually represent requires that one is able to articulate more precisely the relationship between thermodynamics and statistical mechanics, but also the relationship between the theories and reality.

Going further with thinking of this understood as a case of epistemological emergence I still think that emergence is not necessarily the most precise and nuanced way in which Definition 1 should be identified. Even though one can show that it is impossible to predict them directly from the underlying theory of statistical mechanics, I think that this case is different from other (more typical) cases where emergence is argued for. Because, we know what is missing in order to connect the lower-level description to the higher-level property, namely the infinite idealization. Liu's argument does not only state that phase transitions, a property of finite systems, are not reducible to the microscopic theory of phase transitions. It also states that it *is* reducible to an infinite system. It this sense, we know how they could occur within our theoretical framework of statistical mechanics if allowing for the thermodynamic limit to be applied. As described in section (4.1), this point relates to idealizations and approximations in physics, and in this case the question about if the thermodynamic limit can be justified in particular. While it is true that there is a certain sense of irreducibility involved between the higher-level and lower-level description of phase transitions which could be sufficient in order to claim that the

[3]Batterman does not use this term, ontological emergence, himself.

thermodynamic definition of phase transitions represents a case for epistemological emergence, to use the word emergence about this is generally imprecise. Recall the definition of intertheoretic reduction given in (2.1.3). To state that phase transitions are not reducible to statistical mechanics follows from the strongest interpretation of reduction, homogenous reduction. The less strong version of intertheoretic reduction, inhomogenious reduction, permits additional assumptions in the reducing theory in order to connect it to concepts only appearing in the theory to be reduced. In this context, one could ask if the phase transition example rather should be identified as somewhere in between a weak sense of emergence and a weak sense of reduction in the way that Definition 1 is reducible to statistical mechanics but first after taking the thermodynamic limit the system. Allowing for the use of the infinite limit is of course a conceptual problem, so it is not obvious that it can serve as a legitimate additional assumption in statistical mechanics, but it seems even more appropriate to think of this as related to (or caused by) the (complicated) intertheoretic relationship between thermodynamics and statistical mechanics and issues related to idealization in science rather than a clear case of irreducibly.

5.1.2 Qualitatively Different Physical Properties and Emergence

Following the same procedure as above Humphreys' argument in section (4.2) is investigated in this section. In this argument, the emergent property argued for is not the phase transition it self, but more precisely the new phase that the transition gives rise to.

The Case for Emergence

Recall that Humphreys account for emergence rests on the evaluation of the presence of his own four features. These are not necessarily in conflict with Kim's doctrines, but they are less specific, at least the way Humphreys applies them to phase transitions. In the former approach the single issue raised by the necessity of an infinite number of particles alone leaded to the case for emergence. In contrast Humphreys identifies several different aspects associated with the phase transition as emergent properties. Regarding the characteristic about the whole and its parts, both liquidity and solidity, are holistic properties as they result from a composition of their constituents. But additionally Humphreys identifies liquidity and solidity as emergent properties due to that they represent qualitatively different properties at the beginning and the end of the process, the phase transition. This is due to the change from order to disorder (or the other way around). The state after the transition is claimed to be autonomous and novel compared to the old state. As I interpret Humphreys, both vertical (parts and whole-relation) and horizontal (same "level") versions of emergence are exemplified. The autonomy and the novelty of the emergent property are results of horizontal emergence, while the holistic property is vertical. It is not completely obvious how to connect the terms unpredictability, irreducibility and unexplainability to this framework, at least not in a formal way.

But irreducibility in the sense that, the property occurring after the phase transition is not reducible to the one it arises from could potentially work.

Humphreys names the kind of emergence that phase transitions lead to as diachronic ontological emergence and argues that the emergent entity is a physical property resulting from physical processes in time.

Critical Remarks

The way Humphreys treats phase transitions as leading to emergent properties is rather seldom observed in the literature about the topic.[4] While this point by itself cannot serve as serious criticism, the appeal to emergence here seems as a bit too simple or inclusive. This is not primary due to that the characteristics of emergence are not identical to Kim's doctrines. Rather it is about the way Humphreys applies them to this case. The appeal to emergence, which is mainly due to the the apparent qualitatively change in behaviour, e.g., the change from order to disorder, can not by itself be sufficient in order to claim ontological emergence.[5] Additionally, to include emergent entities that do not arise from its microscopic base, but from an previous state of the system is outside the scope of emergence as Kim defines the term.[6]

5.1.3 Universal Behaviour and Emergence

The specific feature of universality appearing only at second order or critical phase transitions has resulted in a new way of thinking of this single aspect of phase transitions in the context of emergence, as Morrison's (and Batterman's) argument(s) showed in section (4.2). In particular Morrison argues that universal behaviour is stable macroscopic behaviour in the sense that this behaviour is not affected by the microscopical details distinguishing one physical system from another system belonging to the same universal class.[7] In this section I will evaluate this argument.

For Emergence

First, regarding the part-whole relation of emergence, universal behaviour is a macroscopic property and can be classified as a higher-level property arising from its microscopic base. Furthermore, to decide whether or not this macroscopic behaviour also involves the other leading ideas of emergence (unpredictability, irreducubility and unexplainability) is a bit more complicated because we actually have a way to predict and/or explain this behaviour. One can start with a particular particle system (represented by its corresponding Hamiltonian) and predict the universal behaviour with the aid of the renormalization group, but the important point is that

[4]The holistic property of the phase itself is however not seldom.

[5]It might be that Humphreys himself is aware of this criticism.

[6]As outlines in section (2.1.4), Humphreys criticizes the classical philosophical idea of emergence for excluding many physical systems which involve horizontal processes in time.

[7]Despite the appearance of the universal behaviour, the scope of this common behaviour is rather limited. As mentioned, there are several features, such as the value of the critical temperature and pressure that actually depend directly on the microscopical details of each system and results in various values of these being system depended.

when performing these calculations, the microscopic details that belong to each system loose their relevance. Since the renormalization group is better identified as a general theoretical framework not connected to any specific microscopic system rather than so-called fundamental theories, the explanation that it provides differs from reductive explanations (which in this context would be a pure statistical mechanical explanation).[8] I will discuss this in more details below.

Critical Remarks

The concept of emergence that universal behaviour at critical points is claimed to satisfy provides is even stronger than the general description of emergence used in this thesis (Kim's doctrines of emergence). Morrison mainly emphasizes that the universal, macroscopic behaviour is emergent due to it being independent[9] of the specific microscopic details of each system. While none of the terms such as independence (or irrelevance or stable behaviour) are explicitly stated as essential characteristics of emergence (neither on the list refereed to in this thesis, nor in the other literature I have read), there might be reasons to think that they could have been there as well or at least that they could be alternatives to the those other leading ideas of emergence. Even if this is true to some extent, I will argue that there is an essential difference between independence and irreduction. Also here it might be illustrative to compare this approach to phase transitions and emergence with the first of the three approaches. If accepting that the fact that one cannot predict phase transitions (including universality) from statistical mechanics as emergence, the main point of the first approach, this shows more specifically that statistical mechanics is insufficient in this task. The meaning of independence, at least the way it is used here, is even stronger than the general understanding of irreducibility. It is not just that we cannot explain the behaviour from the microscopic details (or the particular available microscopic theory), we actually have a method that concretely demonstrates that certain microscopic details are irrelevant.

5.2 What Can We Learn About Emergence From Phase Transitions?

This section wish to answer the second part of the problem formulation:

> *Can the concept of emergence be enlightened or informed by the case of phase transitions?*

The former section was an attempt to describe the case for emergence in each of the three separated topics related to phase transitions. First, regardless of whether

[8] It is not exactly that all the physics of the microscopic level are irrelevant for explaining this behaviour, the so-called general features such as dimensions and short-range forces are actually microscopic features. But the system specific details are not those determining this behaviour.

[9] Should not be confused with being in conflict with the dependency-relation to the physical base.

the positive accounts in each of these sections are valid or not, the fact that there exist so many different ways in which emergence is debated or approached in the context of only one single phenomena, such as phase transitions, might suggest that the term is to frequently applied or that it might be to easy to appeal to.

Furthermore, the critical remarks offered in the former section show that the apparent emergent behaviour in each case do not necessarily satisfy Kim's doctrines:

- *Definition 1*: Even if one give up the aim of figuring out whether the thermodynamic definition of phase transitions today correctly represents the phase transitions we observe, this case does not represent the most obvious case for epistemological emergence either. This is because the incapability of statistical mechanics (leading to unpredictability, irreducibility and unexplainability) to predict the discontinuity in the thermodynamic potential is only partially true. We know how to calculate this discontinuity directly if we allow for the infinite particle system. Obviously, employing such idealization is at least a conceptual problem whose justification should be taken seriously. But it seems more appropriate to think of this issue as related to the (complicated) intertheoretic relationship between thermodynamics and statistical mechanics and idealizations in physics more generally.

- *Qualitatively Different Properties*: The claim that phases are ontological emergent properties (due to the apparently qualitatively change in behaviour - the change from/to order and disorder) is evaluated by an even more inclusive version of emergence than the one specified by Kim's doctrines. While it is possible to sympathize with that this behaviour can be associated with the concept of emergence I am not convinced that ontological emergence is satisfied.

- *Universality*: Morrison's argument for that universal behaviour is emergent behaviour rests on a strong claim of what that should be required by the emergence relation. It is not only the appeal to the insufficiency of the lower-level description to predict these phenomena: Even if there is no reductive explanation of universality we can explain these behaviour, although in an orthodox way. And we are also able to show that there is no need for a more fundamental description (taking microscopic details into account) in order to explain this behaviour. This goes beyond the concept of emergence at least the way it is described here.

Based on the example of phase transitions my suggestion is therefore that rather than appealing to the concept of emergence one could by advantageous use other terms that are able to more precisely capture what is going on in each case. Whether or not this conclusion applies to other examples is unanswered, but the phase transition example at least reinforces the prejudice of the vagueness of emergence.

5.3 Concluding Remarks

Independent of the case of phase transitions investigated, the characteristics picked to describe emergence in this thesis do not, as pinpointed before, correspond to a complete list of necessary and sufficient features that as a whole unambiguously determines which cases that represent emergence and which that do not. Therefore a minimum level of relativity is unfortunately inevitable regardless of whichever conclusion that is made. Due to this, I think that none of the critical points made in the two previous sections by themselves exclude the possibility for that phase transitions could be characterized as emergent entities or properties in one or another way. It is both challenging to prove (or to disprove) that an entity is emergent.

However, and based on the analysis and considerations made in this thesis I will argue that while there are reasons for classifying phase transitions as emergent entities, I am not convinced that they should be or that emergence is the most appropriate term. Many cases of apparently emergent behaviour, such as phase transitions, are quite different compared to one another. One possible objection to this point of view is that the term emergence could be used about different cases in order to express that there is at least a certain kind of similarity between them, even if one has to clarify under which conditions the specific case actually show emergent or similar behaviour. Even if this is true, replacing emergence by other more precise or nuanced concepts would however help avoiding potential confusion, at least if the concept is to be applied in a scientific context.

Chapter 6

Conclusion

In this thesis different arguments defending the view that phase transitions are emergent entities (or lead to emergent entities) have been critically investigated. Phase transitions, the physical phenomena observed as abrupt changes in matter, are today more precisely described by physics, and in particular by the theories of thermodynamics, statistical mechanics and the renormalization group. Phase transitions at the observable level, as well as phase transitions understood in terms of theoretical definitions (and relationships between theoretical frameworks), are claimed to provide evidence for emergence in different ways. This also involves the specific feature of universal behaviour associated with critical phase transitions. In other words, the combined subject of phase transitions and emergence corresponds to a huge topic.

Performing a conceptual analysis in order to answer the question about if phase transitions should be classified as emergent entities or not is a difficult task due to that the concept of emergence lacks a unique description. It is therefore not clear whether this concept could be used to describe phase transitions in one or another way. However, it is argued that the example of phase transitions demonstrates that emergence often is imprecise in this task and that it could be replaced by other more nuanced concepts.

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