Phase transitions in Finite Systems

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1 Introduction

At the close of his second Meditation, Descartes is diverted from intellectual sparring with his all-powerful deceitful demon to consider a more mundane issue. Can he clearly and distinctly perceive the nature of something so simple as a piece of wax? As he places it in his fire its sensible properties of colour, texture and solidity, undergo abrupt qualitative changes, yet it remains the same wax as before. He is forced to admit that none of those sensible properties could be in the nature of the wax itself, and thus he had not clearly and distinctly perceived it after all.

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In picking his example, Descartes chose well. For there are few everyday phenomena that have confounded analysis as consistently as have phase transitions. It was only late in the last century that physics made good progress in understanding many aspects of these changes: how a single collection of molecules can rearrange themselves in such a way that wax can melt, a liquid become a gas, or a piece of iron can become magnetic, while remaining the same materials throughout. It has proved possible to build on existing accounts of many-body systems — statistical mechanics and thermodynamics — to give a comprehensive account of the changes. But this theoretical apparatus continues to provide surprises.

1.1 What is a Phase Transition?

There are clear definitions of what counts as a phase transition within theories of thermodynamics, and there are slightly different definitions within various approaches in statistical mechanics. But it is surprisingly difficult to characterise them in theory-neutral terms. In general, they are marked by abrupt changes in one or more large-scale physical properties of a system, with a small change in some control variable. Descartes' melting wax undergoes a phase transition when its density and other large-scale properties undergo a large change with a small change in temperature. And if we raised the temperature even more, the liquid wax would boil, and the density would undergo an even more dramatic sudden change. We see similar changes in the large-scale magnetic properties of a piece of iron, when we cool it below the Curie temperature and apply a small external magnetic field.

Once we consider phase transitions from within a particular physical theory, we can be a great deal more precise, and can start sorting them into types. Thermodynamics and statistical mechanics both represent phase transitions by non-analyticities in the free energy, as a function of one or more of its thermodynamic variables.

The Ehrenfest categorisation of phase transitions originally took advantage of this definition by grouping phase transitions by the lowest derivative of the free energy which undergoes a discontinuity. Thus first-order transitions (which include melting, boiling and the reversing of magnetic polarisation) have a discontinuity in the first derivative of the free energy with respect to a thermodynamic control variable. Second-order transitions include those at the Curie point of magnets, where the magnetization itself increases continuously from zero, but the magnetic susceptibility undergoes a discontinuity at the Curie tempature. (The magnetization is the first derivative, the susceptibility the second derivative, of the free energy with respect to the applied field.)

The Ehrenfest classification has now been rejected, since its underlying rationale was based in mean-field theory, which has been superseded. Also, it has been found that some of the more complex phase transitions do not fit comfortably into its categories. However, modern approaches retain some of those original distinctions. They begin by sorting phase transitions into two groups: first-order (as with Ehrenfest) and continuous (all the higher-order Ehrenfest). These continuous transitions are then further subdivided according to the symmetries of the phases each side of the transition.

1.2 Two Issues

Recently, a debate has arisen in the philosophy of physics literature on the best way to understand the physical modelling of phase transitions.[1] The controversy centres on the fact that non-analyticities in the free energy of a system are central to the theoretical account of phase transitions, and yet statistical mechanics can only accommodate non-analytiticies in a system with an *infinite* number of degrees of freedom — while physical systems such as Descartes' wax, or a boiling kettle of water are surely finite. In my view, the debate comprises two very separate issues, but the literature has tended to have address them simultaneously, and without distinguishing them clearly.

The first issue is about the relation of theory to real physical systems. The most successful treatments of phase transitions can deal with them only as features of infinitely large systems, and make a central use of this infinite number of elements in order to derive their results. Naïvely, this seems to imply that we have no successful theory of the phase transitions we see around us, since they occur in finite systems. We need an account of how our existing theories may be related to the concrete systems observed in the world. I shall call this the "Idealisation Problem".

A second issue is about the relation between two different theoretical approaches to phase transitions: those based in thermodynamics and those based in statistical mechanics. This second issue can be viewed as a special case of the question of the general relation between those two theories: in what sense, if any, can one be reduced to the other? It has been argued that their respective approaches to phase transitions pose particular difficulties; so I shall call this the

[1]In particular, see Liu (1999, 2001, 2004), Callender (2001) and Batterman (2004).

"Reduction Problem".

I feel that the Idealisation and Reduction problems have been conflated in the existing literature, perhaps because of a belief that statistical mechanics uses non-analyticities to represent phase transitions *only* because of some need to follow the lead of thermodynamics in doing so. Of course such a requirement would lead immediately to a requirement for infinite systems. But as we shall see, putting the issue this way is extremely misleading. For the main reasons for representing phase transitions as non-analyticities are internal to statistical mechanics, and are independent of any need to capture the treatment of phase transitions by thermodynamics. In the rest of this section I shall consider the Reduction Problem and argue that it holds little interest on its own. The remainder of the chapter will then be concerned with the Idealisation Problem, which cannot be dismissed so easily.

1.3 The Reduction Problem

Chuang Liu argued in a 1999 paper that phase transitions provided an example of a genuinely *emergent* phenomenon, in the sense that the treatment provided by thermodynamics cannot be reduced to the treatment of statistical mechanics. In thermodynamics, phase transitions are represented by surfaces, lines and points in the value-space of the relevant thermodynamic variables, at which one or more of these variables is not analytic. Liu judges that 'a rigorous account of phase transitions in purely thermodynamical terms encounters no real conceptual problems' (Liu, 1999, S93). But he also claims that this representation of phase transitions by non-analyticities is 'a feature that any micro-explanations of phase transitions must recover', and goes on to argue that statistical mechanics was wanting in this respect, since under some rather weak assumptions, such non-analyticities cannot appear in a finite system.

Liu notes that the problems can be avoided if we consider statistical mechanics in the 'Thermodynamic Limit' (TD Limit), which involves taking N — the number of particles in the system — to infinity, while carefully preserving their overall density and the interactions between them. In this infinite limit, non-analyticities may appear in the quantities provided by statistical mechanics. But, he contends, the recovery of the thermodynamical representation in statistical mechanics still fails for finite systems. In keeping with his general assumption that a failure of reduction is a signature of 'emergence', Liu calls phase transitions 'emergent phenomena'.

Craig Callender cut off Liu's argument at its first stage, his rebuttal being an instance of the overall thesis of his 2001 paper: that we are often guilty of 'taking thermodynamics too seriously'. In this case, the fault comes when Liu lifts the definition of phase transitions as non-analyticities out from its thermodynamical context, and demands that statistical mechanics must also treat them this way. Callender denies that statistical mechanics has any such obligation and objects to 'this knee-jerk identification of mathematical definitions across levels' (ibid, 550). Rather, he holds that statistical mechanics must be allowed to deal with phase transitions in whatever way seems fruitful by its own lights.

On this particular point, one must surely agree with Callender. By demanding that the same definition be used in each theory, Liu's argument assumes an over-simple view of theoretical reduction. And in any case, the reduction of thermodynamics to statistical mechanics in the classic Nagelian sense has long been recognised to be a project fraught with difficulty.[2]

If anything, it is surprising that statistical mechanics can even approximately reproduce any part of the thermodynamic representation of phase transitions, whether in the TD limit or otherwise.[3] For phase transitions are among the most subtle and intricate phenomena treated by modern physics, and the hard-won theoretical advances have come mainly in statistical mechanics, where they have far outstripped the 'classical' thermodynamic approaches. For example, the phenomena associated with spontaneous magnetisation and supercooled fluids are now sizeable research areas, and neither can be properly understood without a sophisticated statistical mechanical treatment.

Since it goes so far beyond the treatment of thermodynamics, it seems clear that statistical mechanics should be free to develop its own definition and analysis of phase transitions. It would be a ridiculous and artificial restriction to insist on a strict adherence to an old definition for the sake of a reduction project that is already in serious trouble. As such, I shall assume from now on that the Reduction issue may be left aside. When developing new, fruitful methods of dealing

[2]Nagel (1961) is the classic statement of inter-theoretic reduction, though it has been much-criticised. Sklar (1993) gives a comprehensive survey of problems associated with the thermodynamics/statistical mechanics reduction.

[3]Amongst other simplifications, taking the TD limit often quenches thermal fluctuations, which greatly helps the identification of quantities between the two theories. This disappearance of fluctuations in the TD limit might appear to conflict with its use in association with phase transitions. At critical points, it is the presence of fluctuations in the order parameter of the system that drives the distinctive critical behaviour. In fact, in these cases the fluctuations are not quenched by the TD limit, because the correlation length association with the fluctuations also becomes infinite.

with phase transitions within statistical mechanics, or in other frameworks, we should feel no pressure to follow thermodynamics in representing them as non-analyticities.

2 The Need for the Thermodynamic Limit

Despite the claims expressed in the last section, the fact is that almost all of the sophisticated and successful statistical mechanical treatments of phase transitions *do* make use of the TD limit, and they *do* represent phase transitions as singularities. The most successful approaches include mean field theories, Landau's approach, Lee-Yang theory, and renormalisation treatments — all of which use non-analyticies. So even if we follow Callender in dismissing the Reduction issue, we are still confronted with a serious problem. For regardless of how thermodynamics represents phase transitions, statistical mechanics still represents them as non-analyticities in the free energy. And as already mentioned, these non-analyticities do not appear in the free energy of a finite system: only infinite systems can accommodate them. The Idealisation problem is how to relate these accounts to the systems that we see in the world, since they appear to have a finite number of degrees of freedom.

2.1 The Idealisation Problem

I shall now try to set out a clearer statement of the Idealisation problem, and thus of what would count as a satisfactory solution. I will structure the discussion around three questions:

- A Motivation: Why is the thermodynamic limit so useful for theories of phase transitions? Is it indispensible?
- A Definition: What constitutes a phase transition in a finite system?
- A Justification: If our theory of phase transitions does make an ineliminable appeal to the infinite nature of a system, what justification do we have for applying the theory to finite systems?

In practice, physicists do not worry about these questions, mainly because as a matter of empirical fact, quantitative predictions derived for infinite systems hold very accurately for finite systems of "laboratory scale". But it is unsatisfactory for philosophers of physics to merely note as a surprising fact that analyses can be used to model systems for which they are provably inapplicable. We need an account of how this comes about. There has been some interest in addressing this question from philosophers of physics, and as several authors emphasise,[4] our difficulty does look more serious than the *general* worries about relating clean, idealised systems that the theoreticians can consider, to the messy, realistic ones that the experimentalists must observe. For the definition of a phase transition is an all-or-nothing singularity in the free energy, which in no clear sense can be "approached" as N becomes very large. And it is important to realise that the theories really do require a genuine singularity; vague appeals to "steepness" or an "extreme gradient" will not do. For we can find finite systems with extreme gradients in the relevant thermodynamic variables which do not become a singularity as the TD limit is taken: these do not represent phase transitions.

The issue I called 'Motivation', will be addressed in the remainder of this section, where we shall look at the Lee-Yang theory of phase transitions. Using this example, we will see that existing theories do make essential use of the TD limit, but also that there is no barrier in principle to alternative theories that do not appeal to it. Having seen how theories of phase transitions use the TD limit, we can address Craig Callender's suggestion 2001, 547-552 that there is an outright contradiction amongst four statements that could plausibly be made about such theories (§3).

Drawing on the discussion of these points, we will move to the second question of 'Definition', which appears the most urgent; for without a clear definition of phase transitions which applies to finite systems it is difficult to claim that we have a theory of phase transitions at all. In §4, I propose a definition, which allows us to address the third question, of 'Justification': how we can justify applying our best theories to finite systems. Finally, in §5 we apply some lessons drawn from the classical discussion to a suggestion of Laura Ruetsche (2003), that quantum statistical mechanics can provide guidance of how to interpret quantum field theories.

So to start with, we can look at an example of a statistical account of phase transitions as non-analyticities. As already mentioned, mean field theory, Landau's techniques and renormalisation methods each make use of the TD limit, but perhaps the clearest example of the ineliminability of the infinite nature of the

[4] Examples are found in Callender (2001, 550), Liu (1999, S100), and Batterman (2004, 13-14). (Batterman is especially concerned with the *singular* limits that appear at continuous phase transitions.)

models is to be found in Lee-Yang theory (Yang and Lee, 1952). The details are found in standard textbooks (e.g., Thompson (1972, 85-89), Reichl (1980)), and only an outline sketch need be given here.

2.2 The Lee-Yang Theory of Phase Transitions

Although the Lee-Yang theory is a very general approach, we can illustrate it with a concrete example. Consider a simple model system of a large, but finite number of spins in thermal contact with an external reservoir. The total energy E can take values $n\epsilon$, where $n = 0, 1, 2, ..., N$, where N is the total number of energy levels and ϵ is the interaction energy between the spins. If we write the number of microstates corresponding to the nth energy level as $g(n)$, the canonical partition function is given by:

$$Z_N(\beta) = \sum_{n=0}^{N} g(n) e^{-\beta n \epsilon} \tag{1}$$

where $\beta = \frac{1}{kT}$, the inverse temperature. We make the change of variable $z \equiv e^{-\beta\epsilon}$, which allows us to factorise the polynomial

$$Z_N(z) = \sum_{n=0}^{N} g(n) z^n = \kappa \prod_{r=1}^{N(V)} \ln\left(1 - \frac{z}{z_n}\right), \tag{2}$$

where z_n are the N zeroes of the partition function, and κ is a constant which we will ignore in what follows. Since all coefficients in Equation 2 are positive, the z_n will lie away from the physical values of z, which are on the positive real axis.

To analyse the locations of the zeroes in more detail, we define the complex generalization of the free energy:

$$h_N(z) \equiv \frac{\ln Z_N(z)}{N} = \frac{1}{N} \sum_{n=1}^{N} \ln\left(1 - \frac{z}{z_n}\right) \tag{3}$$

and note that a Taylor expansion of $h_N(z)$ around a point $z \neq z_n$ has a finite radius of convergence, given by the distance of the nearest zero from z. Therefore $h_N(z)$ can be differentiated infinitely many times in any region that does not contain any zeroes, which means that within such a region there will be no non-analyticities in the partition function nor the free energy. Therefore, for any point z_0, there can be a phase transition only if there is a zero in a region arbitrarily close to it on the complex plane. For finite N, there will be a finite number of zeroes, so there will be no phase transitions except at the points z_n themselves. And we have already seen that these lie away from the physical values of z on the positive real axis.

We now want to see how a phase transition might develop in the limit of infinite N. Here we assume that the limit:

$$h(z) = \lim_{N\to\infty} \frac{\ln ZN(z)}{N} \tag{4}$$

exists, and that we can write

$$h(z) = \int dz'\rho(z')\ln\left(1 - \frac{z}{z'}\right) \tag{5}$$

where $\rho(z')$ is the local density of zeroes in the complex plane.[5]

Analysis of this expression can show us where the local density of zeroes is positive. For systems such as our simple model, we obtain a curve C that "snips" the real axis.[6] And so at the region where the curve meets this axis, we have the possibility of a non-analyticity, and therefore a physical phase transition.

What is more, the Lee-Yang method provides a classification of phase transitions, according to the line density of zeroes along this curve C. First-order phase transitions are characterised by the line-density remaining non-zero where C crosses the real axis. But for continuous phase transitions the line density goes smoothly to zero as the curve approaches the axis, and we find no discontinuity in the first derivative of the free energy (though there may be discontinuities in higher derivatives).

This sort of analysis of the density of zeroes in the complex plane, and thereby the nature of the singularities in the free energy, tells us a great deal about how the derivatives of the free energy behave in the TD limit. Since in statistical mechanics, macroscopic quantities are obtained from derivatives of the free energy, this in turn yields information about the properties of a substance as it approaches a phase transition. These predictions can be tested against experiment (albeit on a finite system!) and are found to be remarkably successful.

[5] Ruelle (1969) examines rigorously and generally the conditions for the existence of the TD limit.

[6] Thompson (1972, 85-9) provides an analysis of the shapes of C for some realistic models. Blythe and Evans (2003) give a pedagogical account of Lee-Yang theory, before considering how the techniques can be extended to nonequilibrium cases.

Yet the Lee-Yang analysis also shows clearly that a phase transition — defined as a discontinuity in the free energy — cannot appear in a finite N system of the type considered. What is more, this lack of non-analyticity can be shown under some fairly weak assumptions, which cover a large variety of systems.[7] Yet all the melting and boiling we see around us occur in finite systems. This seems to doom our theoretical account to irrelevance, since it provably does not apply to the phase transitions we observe.

2.3 Some Roles of the Thermodynamic Limit

If we accept (from §1.3) that it is not just from a desire to reproduce the thermodynamic analysis that we model phase transitions as non-analyticities in the TD limit, we must look for other motivations. Discussions tend to focus on a single motivation as *the* reason for its use. But choices vary. Of the authors mentioned so far: Callender focuses on several mathematical conveniences that it allows,[8] Batterman concentrates on its provision of an analysis of singular limits,[9] and Liu on the mathematical rigour it provides.[10]

I feel that settling on one exclusive choice of motivation is a mistake: rather, the TD limit plays several distinct roles in theories of phase transitions. Here I shall separate three, and though I make no claim to comprehensiveness, it appears that much would be lost by ignoring any of them.

[7] Emch and Liu (2002, Ch.12) have a detailed discussion with a rich resource of references. It should be mentioned that some mean field approaches do evade the assumptions that go into such proofs. Nevertheless, most MFTs do still apply the TD limit in any case.

[8] Callender (2001, 549-552). He also makes some puzzling comments about the vanishing of thermal fluctuations in the TD limit. While the neglect of these fluctuations may be important for the Reduction problem, their significance is not so clear for the Idealisation problem. For in the case of critical phase transitions it is these very fluctuations that grow in range, cause the failure of mean field theory and necessitate the use of RG techniques — but both the demonstration of this failure, and the RG techniques themselves, also use the TD limit.

[9] Batterman (2004): a focus I think misplaced for the reasons elaborated in §3.2.

[10] In Liu (1999) he focusses on the need to rigorously derive singularities, and concentrates on the neglect of fluctuations, though here he seems motivated by the Reduction issue. In a later article (Liu, 2001) he concentrates more on the 'accentuation or exaggeration of the corresponding physical properties by neglecting or filling out negligible differences' by which I take him to mean what I call *seclusion* below. A joint paper with Gerard Emch mentions its use in discarding surface effects (Emch and Liu, 2005), and their jointly authored book separates out several more examples of mathematical and physical motivations (Emch and Liu, 2002, 394-6).

2.3.1 Mathematical Convenience

Those who hold that the TD limit is *practically* essential, but foundationally unimportant, tend to motivate its use from mathematical convenience. They grant that physicists use the thermodynamic limit, and that they appeal to the singularities that arise there, but hold that this is just because it makes their calculations easier. In the first place, it is often easier to cope with infinite sums than large-but-finite ones, and it is often possible to simplify matters further by replacing sums with integrals. It is also possible to identify non-analyticities even when we cannot provide exact solutions; the appeal to the line-density of zeroes we saw in Lee-Yang theory is just one example of the powerful geometrical and topological techniques that can be brought to bear.

If mere mathematical convenience were the only reason for the deployment of the TD limit, the whole issue would be of little foundational or philosophical interest (except perhaps as a vivid example of the powers of idealisation, or of the difficulties in inter-theoretic reduction). All that would be required would be a demonstration that a theory using the TD limit gave the same result as the "inconvenient" analysis of the finite case. Experimental success would go a fair way towards such a justification, and for more reassurance, we could compare some 'toy' cases where both finite and infinite results are obtainable. But we are not in this situation; our problem is not that theories of finite phase transitions are mathematically inconvenient or impractical, it is that they do not exist.

2.3.2 Seclusion

A very different set of motivations stem from a need to isolate and separate out distinct phenomena occurring simultaneously at the point of a phase transition. We analyse phase transitions by examining the partition function or free energy of a system, but these functions will be made up from many contributions: some related to the effects of the phase transition itself, but many of them unrelated. We want to remove as many irrelevant contributions as possible, so that the phase transition itself can be recognised apart from extraneous effects. I shall call this practice 'seclusion.

This second motivation has long been recognised in the philosophy of science as a species of idealisation distinct from motivations of mathematical power. It has been with us at least since Galileo's separation of the horizontal and vertical components of a projectile in order to exhibit separately its accelerated and inertial motion. (It may well be older, but McMullin (1985) argues that Galileo was novel in applying the technique, which he calls — perhaps misleadingly — 'causal idealization').

One good example of seclusion is that taking the TD limit automatically discards complicating features such as 'surface' or 'edge effects'. Consider a lattice system of finite extent with contributions to the partition function coming from all sites. The contributions of those at the edges and surfaces will be markedly different to those nearer the centre of the sample, since any short-range interactions will be affected due to their different arrangement of neighbours. In the TD limit, the whole body can be treated as 'bulk', and the surface effects vanish.

We shall see later (§4.3) how "cross-over" effects can separate different categories of phase transitions in the TD limit, and many other seclusion effects appear there. It is in infinite systems that we can distinguish the features that are definitive of phase transitions, as well as distinguishing different types in a systematic classification. However, this does not *imply* that a theory dealing principally with the infinite case should be inapplicable to finite systems: it merely suggests that some work needs to be done to fill the gap; and of course, that is one of the problems with which we are concerned.

2.3.3 Structure

A third motivation for considering the TD limit is that it introduces new mathematical structure to our theories: a structure which plays a more fundamental role than "merely" increasing convenience. Rather, it introduces qualitative distinctions which would not otherwise be available and may be essential to give an adequate theoretical. For example: Robert Batterman insists that theories must recognise the existence of what he calls 'physical discontinuities' (Batterman, 2004) at phase transitions. This demand can be interpreted as requiring that the clear qualitative distinction between physical phases must be reflected directly by some clear qualitative distinction in our mathematical representation of different phases. And such a distinction is not immediately available in representations of states of finite systems.[11]

As we have seen, the Lee-Yang theory appeals to a structure which emerges only as the TD limit is taken — the line-density of zeroes in the complex plane. Other theories provide the required structure in very different forms. Perhaps the most striking examples appear in algebraic approaches to quantum statistical

[11]But see §3.1, where we reject Batterman's further claim that these physical discontinuities must be represented by mathematical discontinuities.

mechanics, where distinct phases of an infinite system are represented as unitarily inequivalent representations of the algebra of its observables (Sewell, 1986, Ch.2). Yet for a finite system, the Stone-von Neumann theorem assures us that all such irreducible representations are unitarily equivalent. So again, without the TD limit our theoretical account does not provide enough structure to distinguish more than one phase. We shall return to this in some detail in §5.

Again, it is perfectly possible that this extra structure can be supplied in some other way than by introducing an infinite system. For example, Lev Landau's approach to phase transitions involves introducing an *order parameter* that expresses characteristic features of each phase, and it seems that one could appeal to attributes such as its sign (when a scalar) or direction (when a vector) to express a qualitative difference between phases. In fact, Landau's approach does use the TD limit and appeals directly to non-analyticities, classifying phase transitions by the lowest order of derivative of the order parameter that contains a discontinuity (Landau and Lifshitz, 1959, Ch.8), but there seems no *a priori* reason why the alternative would not work.

Each of these three roles — convenience, seclusion, and structure — are significant in themselves. While they appear independent of one another, they are all satisfied by the idealisation of taking the TD limit. Of the three, the first appears to be at most a motivation of 'mere' practicality, (though for a working physicist it is of course quite sufficient in itself.) The second and third appear of more foundational importance, and I shall focus on them in what follows. However, it is important to emphasise that none of the roles seems to *require* the infinite limit — alternative approaches are not ruled out. But it is striking that the TD limit is able to fulfill all three roles, and to do so naturally. More significant for what follows, a demonstration that a *single* role can be filled without the TD limit is *not* a solution to the Idealisation problem. We require alternatives for all three.

3 An Apparent Paradox

Craig Callender puts the Idealisation problem in sharp relief in his 2001 paper by presenting four jointly contradictory statements about phase transitions, reproduced (and re-ordered for later convenience) below:

1. Phase transitions are governed/described by classical or quantum statistical mechanics (through Z).

2. Real systems have finite N.

3. Phase transitions occur when the partition function Z has a singularity.

4. Real systems display phase transitions.

Once we add the theorem that a partition function Z of a finite system cannot display a singularity, the four are contradictory. And it is possible to classify attitudes to the nature of phase transitions by looking at which of these statements are denied. In the rest of this Section, I shall examine the consequences of denying each of the statements on Callender's list, and whether doing so can be counted a satisfactory solution to the Idealisation problem. Surprisingly (perhaps), it is possible to find advocates for rejecting of each one of his statements.

3.1 Deny Statement 1: Declare that phase transitions are not governed/described by classical or quantum statistical mechanics

The most straightforward approach is to take our apparent paradox at face value. Ilya Prigogine points to it as yet another failure of reductionistic approaches to complex phenomena: phase transitions are 'emergent properties', a term he uses in a very strong sense, to mean that they are not derivable from known laws of quantum mechanics or classical physics. Accordingly, he holds that phase transitions are insufficiently described by the theories we have been considering, and holds that genuinely new law-like behaviour appears in systems large enough to exhibit such phenomena (Prigogine, 1997, 45).

Since Prigogine has long been engaged in a research project to discover emergent laws across many areas in physics, he draws this conclusion with a great deal more readiness than would most physicists or philosophers. I feel that this straightforward denial of the scope of present physical theories is an extraordinary move to make, given that our paradox started from the striking *success* of statistical mechanics in modelling phase transitions. Our problem is to understand the relation between the infinite methods it uses and the finite systems it models so faithfully. This problem is not touched by trying to deny that any such link exists.

Both Batterman and Liu can be read as considering rather less extreme variations on this position. Liu's conclusion in his most recent article (2004) is that neither the Ising spin models nor the TD limit are 'realistic' in that they do not accurately represent the structure of real systems. But these two deficiencies somehow compensate for one another: 'It seems that by introducing two radically unrealistic idealizations — the Ising lattice and the thermodynamic limit — one is able to do better [than a more realistic approach]' (Liu, 2004, 256). However, it is not entirely clear that Liu equates the 'unrealistic' treatment of statistical mechanics with a straightforward failure of description. It is equally possible to read his statement as marvelling that such an *a priori* unpromising approach gives such accurate results. In any case, Liu gives no explanation of how the compensation is supposed to work, and however we interpret his position, he gives no clue as to how the theories achieve their empirical success.

Robert Batterman suggests that the existence of phase transitions forces us to accept the existence of what he calls 'physical discontinuities'. These are physical quantities which really do undergo discontinuities 'out there' in the world. So he interprets the singularities suggested by the mathematics in a very direct way. As examples he offers the qualitative difference between phases, and also one which he discusses in greater detail, the breaking of water into droplets. In both cases, he holds that the singularity is 'physical'.

> ... it surely does seem very plausible to describe the breakup of water into droplets as a genuine physical discontinuity. 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) in the same way we see a stream of fluid break apart. But that, by itself, does not show that there is no genuine physical discontinuity in the thermodynamic system.
>
> My contention is that thermodynamics is correct to characterize phase transitions as real physical discontinuities and it is correct to represent them mathematically as singularities. Further, without the thermodynamic limit, statistical mechanics would completely fail to capture a genuine feature of the world. Without the thermodynamic limit, in fact, *statistical mechanics is incapable even of establishing the existence of distinct phases of systems.* (Batterman, 2004, 12-13, italics his)

Batterman appears to be siding with Prigogine in insisting that statistical mechanics is actually *wrong* in failing to accommodate phase transitions as physical distincontinuities in finite systems. For he seems to claim the following: a physical discontinuity can be 'seen' as the density of water boiling in the tea kettle instantaneously jumps from one value to another, and so statistical mechanics is inadequate if it fails to represent this discontinuity in any finite system.

I admit to some uncertainty as to how to interpret Batterman's 'physical discontinuities', and it is helpful to disambiguate his thesis into two claims, one markedly stronger than the other. The weaker claim is that there are important features of the physical world that are represented by discontinuities (or more precisely, by non-analyticities) in the mathematics used by our best theories. Since our ability to represent these features would be lost if we gave up using the TD limit, the limit is essential. The stronger claim adds to the first that the features represented by the mathematical discontinuities are 'real physical quantities' undergoing 'real physical discontinuities'.

In so far as I understand Batterman's terminology, the stronger claim appears untenable. For it is possible to recognise the existence of distinct phases and the transition between them without being forced to accept that any physical quantity undergoes a discontinuity. The most straightforward alternative would be to recognise that phase transitions take a finite time, during which the water belongs in no definite phase. This could be implemented in a variety of ways, but one would be the following. Let us consider a finite sample of water, and examine its density as a function of time as it boils. Certainly, there is a range of densities over which we are happy to call it a liquid, and a range of densities over which we happy to call it a gas, and further that there is a discontinuous 'gap' between these two ranges of densities. We can certainly recognise a 'physical discontinuity' in this sense. However, this does not mean that there is any particular sample of water whose density must 'jump' across this gap instantaneously when the water boils.

Further details would vary according to inclination, but one option would be to hold that for the sample of water as a whole, neither the terms 'liquid' and 'gas' are relevant. Alternatively, we can hold that there is local variation while boiling, with some areas being liquids, some gases (until we get down to some scale, at which point these terms fail to apply).

I should clarify that I see no *a priori* reason to deny the possibility of physical discontinuities. Indeed space, time or any other physical quantity may be discrete, in which case they might be very common indeed. However, their existence should not be demonstrable by observing — say — water boiling in a tea kettle. We need an account of phase transitions that would accommodate this behaviour, even if the world contained only continuous physical quantities.

If we reject Batterman's stronger claim, then we are still free to consider the weaker one on its own. His claim then is that without discontinuities, the orthodox statistical mechanical techniques fail to 'capture a genuine feature of the world'. The weak claim leaves aside the issue of whether these 'genuine features' are themselves discontinuities in physical quantities, but they are certainly *something* physically significant, and they need to be represented by any empirically adequate theory. The most obvious way to implement this would be to replace the orthodox procedure for constructing a partition function for a finite system. Rather than sum over a finite number of degrees of freedom, we replace any finite sums by infinite ones. This approach might be in keeping with the actual practice of physicists, but it leaves unanswered all the mandatory questions identified in §2.1. Namely: How can it be justified? What definition can we give for a phase transition in a finite system? As such, Batterman's weak thesis on its own is not an answer to the Idealisation question, and we need to choose another path.

3.2 Deny Statement 2: Declare that real systems do not have finite N

A second way of dealing with our problem is to hold that, contrary to appearances, real systems really do have infinite N. That is, physical systems undergoing phase transitions either have an infinite number of parts, or in some other way acquire the infinite degrees of freedom necessary to support a discontinuity in the free energy.

A direct approach would be to point out that since no real system is completely isolated, the modelling of a finite system with one of infinite extent reflects the fact that the system is always coupled to the rest of the universe.[12] Emch and Liu (2005) can be read as advocating such an approach, with the justification that it is the "least of all evils". They point to the infinitely insulating walls or infinite distances that are implicit when we consider a perfectly isolated finite system, and conclude: 'unless specific surface or boundary effects are of interest, taking the infinite limit is (from a philosophical point of view) more sensible than not taking it'. I would suggest that only from a *practical* or *physical* point of view is it more sensible. From a philosophical point of view, taking the infinite limit represents a far more radical step. For the idealisations involved in postulating completely insulating walls involve neglecting small external perturbations that become smaller as we consider increasingly isolated systems. This limiting procedure is in contrast to the singularities, which are not 'approached' in any simple way as the system becomes larger. In any case, it is not an acceptable defence of a position merely to point out that an alternative also has its problems.

More generally, it is hard to see how such suggestions can provide a satisfactory solution to the Idealisation problem. For example, to provide a definition of a phase transition we do not merely need to show the possibility of non-analyticity, but also that non-analyticity appears at the points of phase transitions, and *only* at those points. Coupling the system to a large number of degrees of freedom makes discontinuities in $\mathcal{F}$ *possible*, but for an adequate theory, they must appear

[12]If we want to reserve judgment about the size of the universe (not to mention considerations of locality), an alternative route to the same goal would to claim that any system can acquire an infinite number of degrees of freedom from interaction with a continuous field of some kind. Classically, this could be the electromagnetic field, but we could also point out that at a quantum level, all matter ultimately has a field-like nature.

at the right places and times. For example: consider two kettles next to one another: in one the water boils, in the other it does not. We must guarantee that the non-analyticity is in some way associated with the first kettle. It cannot 'leak' over to the second kettle, since there is no phase transition occurring there. That is, our non-analyticities must be tied to the finite systems involved in each phase transition. It is difficult to see how such a satisfactory justification could be conjured from an appeal to coupling to the rest of the universe, or to some electromagnetic or quantum field.

But we can modify our denial of the finite nature of the systems to yield a more subtle suggestion. Batterman's weaker suggestion identified in §3.1, might be read as recommending such an adjustment. He might not actually doubt that real systems are made up of a finite number of particles, but he certainly demands that they be 'characterized' using an infinite N.

> I want to champion the manifestly outlandish proposal that despite the fact that real systems are finite, our understanding of them and their behavior requires, in a very strong sense, the idealization of infinite systems and the thermodynamic limit. (Batterman, 2004, 9)

Perhaps the best way to implement Batterman's proposal in Callender's terms would be to modify Statement 2 to: "Real systems have finite N, but to describe them, statistical mechanics must model them as infinite."

I have some sympathy with an alteration in this spirit, but have difficulty with the motivations that Batterman gives. He argues that the ineliminability of infinite limits stems from situations in which the relevant limits are *singular*, that is: when a small parameter being taken to zero describes behaviour that becomes markedly different as the limit is approached.[13]

[13]Batterman begins his article (§§1-3) by considering the relation between theories (the Reduction problem), and there he appears to use singular limits only as a metaphor for a new approach he recommends for intertheoretic reduction. However, his arguments are addressed to the Idealisation problem in the remainder of the paper, and there he appeals to singular limits in a literal sense.

However, these singular limits that Batterman appeals to do *not* appear in all phase transitions, only in some cases such as critical points. There is little space here to discuss the relationship between non-critical and critical phase transitions, and to do so would be to wander from our main theme.[14] But singular limits cannot be the key to understanding why the TD limit must be used. For the theories which adequately represent phase transitions (both critical and non-critical) make a central appeal to the TD limit, whether the limit is singular or not.

Instead, let us agree with Batterman that the use of the TD limit is ineliminable, while reserving judgment on his diagnosis of singular limits as the root cause. This brings us back to the main problems, to definine phase transitions in finite systems and to justifying their application of our best theories. Batterman says little about the details of a definition, but the rest of his article is concerned with providing a justification for infinite idealisations. He illustrates these with a set of examples drawn from hydrodynamics. When a stream of water breaks off into drops, the shapes of the "neck" and of the drops are *universal*: they remain the same across many different kinds of fluid, which nonetheless differ in their microscopic structure. Batterman argues that if the microscopic details of the fluid make no difference to their large-scale features, it might be justifiable to replace a particulate body by a continuum.

For the special case of critical phase transitions, there appears to be hope of a

[14]For more details, see the discussion of different varieties of phase transition in Mainwood (2006, Ch. 3), but a few brief comments seem in order. At a *critical* phase transition, a microstructural property called the *correlation length*, ξ, also diverges to infinity. This ξ is a measure of the range of the correlation of fluctuations. Since mean field theories neglect the correlation of such fluctuations, they fail near critical points (in less than four dimensions for the Ising model), and a mean field account of the critical phenomena is seen to be inadequate. Renormalisation introduces a systematic scheme for reducing the degrees of freedom, utilising a transformation that 'traces them out' while accounting properly for the diverging correlation length, and that does not fail near the transition, but instead gives accurate predictions for quantities such as the critical exponents. The main point for our purposes is that the failure of the mean field approximations is *not* directly connected to the necessity for the infinite limit, but rather to the diverging correlation length.

similar approach. Some critical phenomena are also universal: the same large-scale effects occur in systems with widely varying micro-physical details. Renormalisation techniques provide an account of this universality, and an argument could be made that a sufficiently judicious replacement of a finite spaced lattice with a continuum might leave untouched the large-scale physics that we observe in phase transitions.

But worries immediately arise. First, we do not seem to dispense completely with an infinite system. As mentioned in §2, renormalisation techniques *start* with infinite N models, and then demonstrate that the physics below a certain scale can be neglected.[15] This suggests only that details below a certain scale are irrelevant, not that the infinite nature of the system can be disregarded completely. A second concern is that the phenomenon of universality occurs only near critical points, not at all phase transitions; and even there, not all properties associated with phase transitions are universal. For example, the temperature at which a critical phase transition appears is *not* universal. As far as I understand Batterman's suggestions, his justification for 'screening off' small-scale physics would not hold for such properties, so there would be no reason to trust the predictions of the theory.

3.3 Deny Statement 3: Declare that phase transitions do not only occur when the partition function has a singularity

This is the course recommended by Craig Callender, and is also one of the options considered by Chuang Liu. Callender diagnoses our temptation to accede to the statement as stemming from our wish to directly import definitions from

[15]The particularly interesting case of finite-size crossover is addressed in §4.2.

thermodynamics to statistical mechanics, but as he points out: 'the fact that thermodynamics treats phase transitions as singularities doesn't imply that statistical mechanics must too.' But in diagnosing this motivation, Callender is engaging only with the Reduction problem. Simply denying Statement 3 leaves the theory of statistical mechanics without a good account of finite phase transitions, indeed it leaves us unable to recognise their existence. Callender holds that finite phase transitions must be governed by analytic partition functions, which 'in some sense approximate a singularity', but gives little idea of what this sense is to be.

The most obvious move would be to assume that a sufficiently extreme gradient in the free energy could represent a phase transition. However, this cannot be the whole story. The Lee-Yang theory, in common with other treatments, requires a genuine discontinuity, not just an extreme gradient in the free energy. We can easily construct finite systems with extreme gradients in their free energy that do not develop into discontinuities when the TD limit is taken; these do not signify genuine phase transitions.

Liu (2001, 2004) is also worried by the difficulties presented in filling out Callender's 'some sense' of approximation, because he feels that this only makes sense when one can point to an asymptotic limit which ends at a phase transition. Liu draws a contrast with how we might justify 'applying calculus to *almost* continuous bodies (i.e., those which contain a large number of very small particles of finite mass)'. He judges that we are correct to do so, because it is meaningful to say that $\delta M/\delta V$ approaches dM/dV, as $\delta M \to 0$.[16] Thus there is a clear sense in which one quantity approximates the other for 'almost continuous bodies'. However, this is in contrast to the case of the thermodynamic limit:

> Until the limit is reached, the pressure or free energy of any macrosystem is analytic. The non-analyticity is not at all asymptotically reached

[16]Of course, this is not a rigourous approach to justifying the application of calculus to physical systems, but it serves to illustrate Liu's argument.

> by the process of taking TL [the Thermodynamic Limit]. At no stage of this process is non-analyticity (representing a phase transition) roughly or approximately defined. (Liu, 1999, S103)

Here Liu brings up an important consideration, but a further distinction needs to be made. Consider Liu's 'almost continuous' body. There are at least two ways to regard his justification for applying calculus to it. The first is the one that Liu discusses: we consider the quantity $\delta M/\delta V$ for the particulate body, which can be directly interpreted as a physical quantity. Postulating a differentiable function $M \equiv M(V)$ and considering its derivative dM/dV, we can then show that $\delta M/\delta V$ is very well approximated by dM/dV as δM becomes very small. This provides us with a justification for making the substitution $\delta M/\delta V \approx dM/dV$ throughout our equations. In this first approach we aim to represent a realistic physical system, but then approximate some of the terms in our mathematics.

A second way is to argue that in regard to the behaviour of the body that we are interested in, it would be as well to consider a continuous substance rather than one made up from particles. We therefore consider this idealised physical situation rather than the original: modelling a continuous body rather than an atomistic one. In this case, the quantity dM/dV is treated as representing a physical quantity, albeit one connected to a fictional, unrealistic situation. To justify this procedure, we need some argument that the substitute system will share the behaviour we are interested in. To make such an argument there is no sense in which the particulate body need 'get asymptotically closer' to the continuous one. And this is so, even if we do appeal to the fact that $\delta M/\delta V \approx dM/dV$ for small δM.

This distinction is a well-known one, and versions have been drawn in many different contexts, and under many different names. Butterfield (2006, 24-5) and Teller (1979, 348-9) agree in calling the first 'approximation' and the second 'idealization'. McMullin (1985, 264n) separates similar procedures under the headings:

'construct' idealization and 'causal' idealization.[17] I shall continue with Butterfield and Teller's terminology in what follows.

In many cases, the choice between idealisation and approximation makes little practical difference, because we often find that the justification we need to supply for each procedure is very similar. We have already seen in Liu's example that the small difference between $\delta M/\delta V$ and dM/dV may be used to justify either approximation or idealisation. Or consider an almost force-free body such as a hockey puck moving on ice. We might either consider dropping some of the smaller force terms from our equations (approximation) or replacing the whole problem with consideration of a genuinely force-free one (idealisation). In both cases the equations we consider will be the same, and the justification for each comes from the negligible differences that these force terms make to the results we are interested in. For these cases, the idealisation/approximation distinction is of no importance to how a calculation proceeds.

But sometimes the two come apart: and in cases associated with the TD limit, the distinction is often crucial. Callender's 'in some sense' cannot be filled out by considering an approximation: it must refer to an idealisation. In other words: Liu's absurdity of attempting to 'approximate an analyticity with a non-analyticity' (whatever that might amount to), can be avoided if instead we idealise a finite system with an infinite one. For it is legitimate to replace a finite system with an infinite one, and *then* to consider what sort of features of the finite systems might correspond to the non-analyticities that appear in the free energy of its infinite replacement. Of course we must face the questions of the physical significance of this procedure. Most importantly: what justification can we provide that the replacement will give us insight into the phase transitions of the original? I shall

[17]Other authors draw similar distinctions, Cartwright (1989) uses 'abstraction' for what I am terming 'idealisation', but she is also interested are interested in wider connotations, such as a distinction between "partially true", and "strictly false" idealisations. I would like to avoid these additional considerations.

try to fill some of these gaps in §4.2.

Before we move to consider the next option, we must mention the specialist research programme studying phase transitions in 'small' systems, or those involving gravitational effects, where the TD limit cannot be applied. One advocate of this approach, Dieter Gross, argues that many first-order phase transitions are *not* best understood in the TD limit. He works with an alternative set of definitions, based around the statistical mechanics of the microcanonical ensemble (Gross, 2001). This is a far more straightforward denial of Statement 3 than we have so far considered: Gross simply rejects the whole non-analyticity approach, and suggests an alternative way in which statistical mechanics can model phase transitions. Unfortunately, it appears that these replacement definitions do not give rise to theories with as wide a range of applicability as the orthodox ones. So until Gross' programme develops further, his approach must be seen as a complement, rather than a replacement.

3.4 Deny Statement 4: Declare that real systems do not display phase transitions

Perhaps surprisingly, this is the option that appears to be taken by many physicists, even those who have made great contributions to theories of phase transitions. For example, Leo Kadanoff was the first to propose that the 'scaling' relations seen in critical phenomena could be analysed using a 'blocking' procedure.[18] In his textbook on critical phenomena he writes:

> The existence of a phase transition requires an infinite system. No phase transitions occur in systems with a finite number of degrees of freedom. (Kadanoff, 2000, 238)

[18]Mainwood (2006, Chap. 3) gives more details of his proposals, and how his line of thought was later honed into the techniques of the Renormalisation Group by Kenneth Wilson.

Similar statements can be found in many texts, usually with an associated plea that as the systems we see around us have very large N, they are 'effectively' or 'nearly' infinite. (Of course, as we discussed in §3.3, a discontinuity does not appear at *any* finite N, nor do we get "nearer" to one as N increases.)

Perhaps even more striking is the attitude expressed in a text on the computer modelling of phase transitions (Mouritsen, 1984). These techniques model only a finite array of spins, and one might expect that theoreticians would welcome these as providing a more direct route to real physical transitions than do orthodox techniques, since they reproduce the finite nature of the physical systems. Not in the least; Mouritsen follows Kadanoff in declaring that phase transitions cannot occur in finite systems, and continues:

> Nevertheless, finite systems have *reminiscences* of phase transitions, and systematic [computer] studies of these pseudo-transitions as functions of system size may reveal information about the phase transition in the infinite system. (Mouritsen, 1984, 20, italics his.)

So even in those situations where it is mathematically convenient (indeed, necessary) to model a finite system directly, there is no suggestion that these models can show anything other than a 'pseudo-transition'. Instead, we look at our results as functions of system size, and attempt to extrapolate them to the infinite case. Only when Mouritsen is satisfied that the infinite case would exhibit a non-analyticity, does he consider that we really are dealing with a true phase transition, and only then does he attempt to categorise it and draw further conclusions about its properties (Mouritsen, 1984, 22-26).

The fact that these theoreticians of phase transitions flatly deny that they take place in finite systems, may seem surprising. Presumably, they see kettles boil no less clearly than the rest of us. But the very fact that they feel that their denials are uncontroversial suggests that we are dealing with a matter of words only. The modelling of phase transitions with non-analyticities is a part of their theoretical toolbox, and the term 'phase transitions' has come to refer only to phenomena that fit this definition. Of course a change in reference of the term 'phase transition' does not solve the Idealisation problem, but just changes the form of words in which it must be stated. In usual terms the problem was to relate phase transitions in finite systems to a definition available only in infinite systems. Now we must state it as a problem of relating "nameless phase-transition-like phenomena" in finite systems to "phase transitions", now defined so as to only appear in infinite systems. Likewise, the theoretician's pleas that large systems are 'effectively' or 'nearly' infinite, translate to Callender's statement that the phase transitions must 'in some sense' approximate a singularity. The problems remain the same: the fact that we trust the infinite results to tell us about the finite sized phenomenon remains unchanged, and we still need an account of when this trust is well-founded.

4 Phase Transitions in Finite Systems

Let us review the issues still outstanding. We have a definition of phase transitions common to almost all successful theories of those phenomena. This definition, as well as those theories, apply only to infinite systems. Yet they describe well the phase transitions (or "phase-transition-like" behaviour) of finite systems, indeed this is the main standard by which we judge their success. To avoid a simple contradiction, we could choose to deny any of the four statements presented in §§3.1-3.4: but by just doing so we may leave the important questions untouched. We have seen some reasons for the utility of the TD limit, but still require (i) a definition for phase transitions that we can apply to finite systems and (ii) a justification for applying the theories to them. In §4.1 and §4.2I shall address each of these, and then in §4.3, return to see how the answers cast light on how the TD limit is able to fulfill the roles we identified for it.

4.1 Defining Phase Transitions in Finite Systems

Consider a finite system with N degrees of freedom in a particular state S. Let us denote its free energy as $\mathcal{F}_N(S)$ and its partition function as $Z_N(S)$. And assume that our system is one in that clearly delimited set for which there exists a well-defined procedure for taking the thermodynamic limit. The free energy of that system when the TD limit is taken we can call $\mathcal{F}_\infty(S)$ and the partition function $Z_\infty(S)$. (Naturally, $\mathcal{F}_N(S)$ and $\mathcal{F}_\infty(S)$ will coincide for a system that is already infinite). We have a well-defined criterion for phase transitions in infinite systems, so there is an obvious definition for the finite case.

Definition 1. *Phase transitions occur for a finite system in state S if and only if $\mathcal{F}_\infty(S)$ has a singularity.*

Rather surprisingly, using this definition it is possible to hold on to all of Callender's four statements without contradiction; though only in a Pickwickian sense — it is a "trick" possible only due to his choice of wording. Namely, the singularity referred to in Statement 3 is one not in the partition function Z_N but in Z_∞.

I believe that this definition of a phase transition in a finite system is at least naturalistically appropriate, in that it is in keeping with the practice of physicists. In particular, it accounts for their uncritical reliance on theories of the infinite to tell us about finite cases. For example, it makes some sense of the otherwise odd practice we saw in §3.4, of withholding judgment as to the nature of a phase transition until results are rigorously demonstrated in the infinite case, even if finite results are available.

But from a philosophical point of view the definition looks suspect, for it seems to make the existence of phase transitions a subjective, theory-dependent question, rather than something directly determined by physical facts about a physical system. This worry can be decomposed into two more sharply defined objections: first, that the existence of a phase transition is determined by a counterfactual (indeed, a highly unrealistic counterfactual); and second, that the existence of the phase transition depends on exactly how the system is modelled, or how the TD limit is taken — subjective matters that we can change on a whim. Let us take these in turn.

4.1.1 Phase Transitions are Actual

The thought behind the objection is that properties such as 'is boiling' appear to be an intrinsic property of a given sample of water. And as such, the facts we need to decide whether or not it is undergoing a phase transition should be physical facts, about actual states of affairs contained within — say — a kettle. They should not exist only in an idealised model on a theoretician's blackboard.

This objection is based on a version of a general principle often known as the 'Truthmaker Principle', roughly: that any actually true proposition should be made true by actual facts, real goings-on in the world. Put as a general claim, the principle is both disputable and lacks an agreed articulation (and this is not for a lack of attempts, e.g., Armstrong (1997, Ch.8) and Mellor (2005)). But I shall not dispute the specific version appealed to here. For if we look carefully at Definition 1, we see that all the truthmaking facts *can* be located within the kettle, though we may need to appeal to counterfactuals to apply our detailed theory and decide whether the facts count as a phase transition (and if so, what type). That is, it is facts about the finite sample of water that determine whether or not a phase transition is occurring, and determine whether it is first-order or continuous. However, we find it necessary to appeal to a radically counterfactual circumstance to state these facts in any reasonable way.

There is a strong parallel between this situation and the defense offered by David Lewis in regard to his analysis of counterfactuals, which is held to contravene a similar principle. He defends his analysis, which is made in terms of a "similarity" relation amongst possible worlds, by suggesting that it is the qualitative character of the actual world which determines this "similarity" relation. However, he also defends the ineliminability of the other possible worlds: 'it is only by bringing the other worlds into the story that we can say in any concise way what [qualitative] character it takes to make what counterfactuals true' (Lewis, 1986, 22). Lewis' memorable example was the following: while it is no doubt possible to describe Buenos Aires to a stay-at-home Australian by describing many intrinsic properties of Buenos Aires, it is so much more concise and illuminating to say 'It's like a Spanish-speaking Sydney'.[19]

Returning to the tea kettle, we should realise that it is the character of the finite sample of water that determine the nature of the infinite system that we then consider. When we draw conclusions about the nature of the phase transitions, they are conclusions about the character of the finite sample, but by reference to the infinite model we can express them in concise and illuminating form.

This consideration also blunts the worry that our definitions makes reference to physically impossible circumstances. So long as we are satisfied that the truth-makers are intrinsic properties of the finite boiling water, the physical impossibility of the TD limit does not seem to pose any *further* problem than does the original counterfactual appeal. There is nothing paradoxical about the fact that our clear, concise expression makes reference to a physically impossible situation. Of course it must be conceded that an uncritical consideration of physically impossible counterfactuals might lead us to all kinds of absurd conclusions. We must be cautious,

[19] I thank Jeremy Butterfield for pointing out the parallels with Lewis' position. His 2003 paper contains an interesting note on the genesis of this particular example (24n).

and this is part of the reason why it is so important to take the TD limit in a well-defined manner.

4.1.2 Phase Transitions are Objective

While there exist standard procedures for taking the thermodynamic limit, and rigorous methods to determine whether it is well-defined,[20] these procedures are human inventions, and choices could have been made differently. Even when clear rules are laid down, theoreticians will always be willing to break them, if it proves fruitful for the analysis a particular situation. The definition of a phase transition thus seems arbitrary in a disastrous sense: we can choose whether one is occurring or not by modelling it differently, or taking the limit according a different scheme.

To allay this concern, it should be recognised that it was empirical considerations that have led TD limits to be taken in the way that they are. Over the last century, theories have developed to account for differences and similarities in the phase transitions we observe. We have been led to distinguish first-order vs. continuous transitions; and symmetry-breaking vs. non-symmetry-breaking transitions for example. The particular procedure for taking the TD limit has developed along with the theories, in such a way that phase transitions are defined in good accordance with experiment, and the categorisation is faithful to empirical similarities and distinctions.

If it was found that a different set of methods for taking the TD limit gave a better classification of phase transitions, more faithfully accounting for the experimental observation, it would be adopted. There are good historical examples of such alterations: for example, we mentioned earlier how the Ehrenfest cate-

[20] Ruelle (1969) is the definitive modern analysis of the conditions that allow a TD limit. Emch and Liu (2002, Chs. 11-12) provide a historical and philosophical discussion of the techniques, including the amusing fact that the necessity of the TD Limit was put to a vote at a 1937 conference. The result was not recorded.

gorisation of nth-order phase transitions (n being the lowest order of derivative of the free energy with a discontinuity) was discarded when it was found to exclude transitions where $\mathcal{F}$ diverges.[21]

One final difficulty must be mentioned. Strictly interpreted, the definition I have offered would allow phase transitions to occur in very small systems indeed. A lattice of four Ising spins laid out in a square might be said to have the infinite two-dimensional Ising model as their TD limit, and so could undergo a phase transition. Personally, I think this bullet can and should be bitten, but it can also be easily dodged. To do so, one might add an additional condition that the original finite system must be sufficiently large, or the gradient of $\mathcal{F}_N$ be sufficiently steep, before any change can qualify as a phase transition. This will make the attribution of phase transitions a vague matter in some cases, but we would have no problem producing clear cases on each side of the divide: four atoms of H_2O would not be enough to boil, but a kettle full of it can.

4.2 Justifying the Application to Finite Systems

If the account presented in the last section is acceptable, then we have a definition of a phase transition in a finite system. We are now in a position to move to our last question: how can we justify applying our theories of infinite phase transitions to finite ones? A partial answer can be made by appealing to the design of the TD limit: for the whole point of the limit is to produce an infinite system that would tell us about the statistical mechanical behaviour of the original finite one. More support comes from a simple appeal to empirical success. But it would be advantageous to come up with further justification, and in some specific cases we can.

As an example, consider the phenomenon of *crossover*, an important feature

[21] For historical details, see Domb (1996).

of critical phase transitions. As substances approach a critical phase transition, they typically exhibit behaviour characteristic of one of a small number of *universality classes.* For example, beta-brass is placed in the "Three-dimensional Ising universality class", since it shows critical behaviour associated with that of the 3D Ising model. 'Crossover' happens when a substance appears to show behaviour characteristic of one universality class, but then suddenly changes to another as it is brought even closer to its critical point. One of the triumphs of Renormalisation techniques are that they provide a beautiful explanation of crossover, entirely lacking in older techniques such as mean field theories and Landau's approach.

A feeling for the Renormalisation explanation can be given follows; (full and clear treatments can be found in good textbooks on critical phenomena such as Cardy (1996, Ch.4) or Goldenfeld (1992, 271-280); an outline from a philosophical standpoint is given in Mainwood (2006, Chap. 3)). A condensed matter system can be characterised by the parameters of its microscopic Hamiltonian: interaction strengths between molecules, couplings between an external field and the system, and so on. We can represent many different Hamiltonians by constructing a space coordinatised by all of these parameter values, with each Hamiltonian represented by a point in the space. (Typically, the temperature is also represented as a parameter in this space, so each point represents a system at a particular temperature.)

Renormalisation techniques allow us to examine the near-critical behaviour of such systems by constructing an iterable transformation on this space. The transformation is designed to preserve the large-scale physics of the system, and the resulting system is rescaled so it can also be assigned a point within the space of Hamiltonians. The transformation thus induces a 'flow' through points in the parameter space which preserves all the large-scale physics of the system. There are certain *fixed points* of these transformations, and the properties of some of them (in particular, the *critical* fixed points), can be shown to affect the near-critical behaviour of any system whose flow comes close to them. Crossover occurs when a system's flow approaches one fixed point, but then as it is brought closer, it veers away and as a result, loses the behaviour characteristic of one universality class and takes on another behaviour associated with another.

At critical phase transitions, a quantity known as the *correlation length* diverges. A particular variety of crossover, known as *finite-size crossover*, occurs when the ratio of the correlation length to the system's size determines the fixed point to which the system flows. When the correlation length is small compared to the size of the system, the system's flow is attracted to a fixed point associated with the phase transition of an infinite system. However, as this phase transition is neared, the correlation length grows, becomes comparable to the size of the finite system, and then the flow crosses over to some different fixed point. The upshot is that as a parameter such as temperature is tuned so that a system approaches the critical phase transition, the system exhibits behaviour characteristic of an infinite system, but as the temperature is tuned more closely to the critical point, this behaviour disappears. Usually this is reflected in the 'smoothing out' of the gradients of quantities such as the free energy, so the singularities associated with an infinite system become peaks, which are tall and narrow — but analytic.

Finite-size crossover thus provides a very neat explanation for how a theory of phase transitions which only describes infinite systems, might model finite systems to accuracies well within experimental error. For a correlation length will only approach a system's physical size as it is brought incredibly close to the phase transition itself, well within the tolerance of experimental measurement. And until we enter this regime the critical behaviour will be as though the system was infinite in extent. So powerful is this effect, physicists can be confident that experimental results on finite physical systems should match the theoretical ones taken in the TD limit.

We can give a measure of how striking this effect can be, when we consider the process of extrapolating the results of computer models of a finite number of spins to the TD limit. Computer models of systems as small as $L = 10a$ (i.e., ten spins per side of a square lattice,) have been shown to give results so close to the theoretical results obtained in the TD limit for 2D and 3D Ising systems (Mouritsen, 1984, 21) that little extrapolation is needed.

Here I should admit to some double-standards. In §3.2 I criticised Batterman for offering general accounts of phase transitions which apply only to specific cases. I admit that finite-size crossover also only provides an example of how we might justifying the application of our theories of phase transitions to near-critical systems — it is not a general prescription. And in fact, justifications tend to be made on a case-by-case basis. Where all else fails, large computer simulations of specific systems can give much reassurance that as N gets large for a specific system, quantities such as the free energy converge to the values obtained in the TD limit. These cannot give general proofs, but can provide justification for the use of the theories on a model-by-model basis.

4.3 More on the Roles of the TD Limit

Back in §2.3, we identified three separate roles which the TD limit fulfils. The first, of mathematical convenience, is no doubt dispensible in principle, and with vast increases in computing power, perhaps sometimes even in practice. But it is the other two roles that are of foundational significance: the need to isolate and *seclude* the phenomena we are interested in, and to provide the mathematical *structure* in order to distinguish them into their natural varieties and disregard any unrelated effects. As we shall see in this section, these are not merely practical considerations, and the TD limit fills both roles simultaneously.

Let us start with 'seclusion'. Real, finite, phase transitions are invariably hybrid beasts, with contributions to their partition function or free energy coming from many different effects, and even from different types of phase transition. A satisfactory theory of phase transitions must be able to tease these apart, provide a categorisation, and some understanding of how the effects may combine to produce the effects we see.

One kind of hybrid phase transition occurs in systems very much larger in some spatial directions than in others, and here we can appeal to another type of crossover phenomenon, known as *dimensional crossover*. When we apply the definition offered in §4.1, our first task is to take the TD limit, but in these cases it may be unclear in which dimensions it should to be taken. For example, we might be trying to analyse the transitions of a very thin film of some substance, just a few atoms thick. In this case, it might not be obvious whether we are to take the infinite limit of a two-dimensional or three-dimensional system. But dimensionality has an extremely pronounced effect on phase transitions. Typically, choosing between two and three dimensions is amounts to a choice as to the type of phase transition, or even whether it takes place at all. Thus, we revisit the "subjective" worry of §4.1.2.

Consider the parameter space once more. Both two and three-dimensional infinite systems will have their own fixed points. As the correlation length approaches a scale similar to the thickness of the film, the flow can "cross over" from three to two-dimensional behaviour. Let us say for the sake of argument that both fixed points represent phase transitions, but of different varieties. What we would observe in this case is a substance behaving at first as though were undergoing a three-dimensional phase transition, but then as it is brought closer to the transition point, switching to behaviour associated with a two-dimensional system. To the question of whether the substance is *really* undergoing a phase transition of the two or three dimensional variety, the most natural answer would be that it showed behaviour associated with both.

The crossover phenomenon goes some way to reassuring us that the limited arbitrariness of how the infinite limit should be taken is not a problem — to speak figuratively: even the substance itself seems unsure and crosses over between the two options! But the main point is as follows: the composite behaviour of the finite system can be understood theoretically by looking at the two basic types of transition in the infinite limit, and then look at how they interfere with one another in crossover. Dimensional crossover thus provides further illustration of the indispensibility of the TD limit, both from the need to *seclude* the phenomena associated with phase transitions and also by providing the additional *structure* to separate them cleanly into classes associated with the fixed points (both of the italicised terms being taken in the sense of §2.3).

5 Putting Unitary Inequivalence to Work?

There is a striking feature of the interpretation of quantum field theories: the lack of a unique Hilbert space representation of their canonical commutation relations. This situation prompts various interpretative questions, among them, we must decide which of these representations should be given direct physical significance, whether any are privileged above others. It also suggests that there is no unique quantisation of a given classical field theory.

In a 2003 paper, Laura Ruetsche takes an original approach to such problems. She starts from the observation that the lack of uniqueness arises from the infinite degrees of freedom of the field, and observes that this feature is also present in quantum statistical mechanics (QSM) when the thermodynamic limit is taken. But in the QSM context, there is a better established understanding of the representational work done by inequivalent Hilbert space representations, and she proposes that we should be guided to analogous conclusions in the interpretation of quantum field theories.

In this section, I want to challenge Ruetsche's approach: not because I utterly reject the interpretation she arrives at, but because the reasoning that takes her there is directly undermined by the position taken in the rest of this chapter.

5.1 Algebras and their Representations

The standard way of looking at quantum theories of finite systems is as a *Hilbert space theory.* Such a theory is characterised by the following features:[22]

- The *observables* are associated with the set $\mathfrak{B}(\mathcal{H})$ of all bounded self-adjoint operators acting on a Hilbert space $\mathcal{H}$.
- The *states* of the system are represented by the set $\rho(\mathcal{H})$ of all positive normalised trace-class operators on a separable Hilbert space $\mathcal{H}$.
- For a state $\hat{\rho}$ and an observable $\hat{A}$, the theory associates an *expectation value* $Tr(\rho A)$.
- The *dynamics* of the system can be represented by the unitary operator $\hat{U}_t = e^{\frac{-i\hat{H}t}{\hbar}}$, where $\hat{H}$ is the energy observable. In the Heisenberg picture, this operator acts on the observables, giving the evolution of a state $\hat{\rho}$ over time t as a transformation $\hat{A} \to \hat{A}_t$, where $\hat{A}_t = \hat{U}_t \hat{A} \hat{U}_t^*$.

The standard way of obtaining such a structure is to quantise a classical theory. In fact, there is a rather successful algorithm which we can use to convert a classical theory cast in Hamiltonian form into a Hilbert space theory. This *quantisation algorithm* takes the canonical position and momentum variables (q_i, p_i) and converts them to symmetric operators $(\hat{q}_i, \hat{p}_i)$ acting on a separable Hilbert space $\mathcal{H}$,

[22] In what follows, I take on the notation and approach of Ruetsche (2003), with additional material and discussion taken from Sewell (1986) and Emch (2006).

obeying canonical commutation relations (CCR's) which are related to the classical Poisson bracket. We call a Hilbert space theory that satisfies the scheme, a *representation* of the CCR's, and write one as $(\mathcal{H}, \{\hat{O}_i\})$.

Although it is still orthodox to think of quantum theories as Hilbert space theories, there is an alternative view which arose from the investigation of the realisations of CCRs in quantum field theory. It can be shown that each Hilbert space representation of CCR's gives rise to an abstract C^* algebra, called its *Weyl Algebra*, and that this algebraic structure was independent of the particular Hilbert space representation chosen.[23] The suggestion is that this Weyl algebra could be considered as a theoretical framework in its own right, directly representing the states and observables of the quantum system. And because this alternative representation is unique, it might even provide a 'cleaner' interpretation of a quantum theory, than the Hilbert space theory obtained by the orthodox quantisation algorithm. This *algebraic approach* identifies bounded[24] quantum observables directly with self-adjoint elements of a C^* algebra $\mathcal{A}$, and physical states with functionals ω on $\mathcal{A}$, specifically the linear functionals $\omega : \mathcal{A} \to \mathbb{C}$, which are normed and positive for all $A \in \mathcal{A}$.

The links between the two approaches are strong, for we can *represent* an algebra $\mathcal{A}$ in a particular Hilbert space, by setting up a structure preserving map $\pi : \mathcal{A} \to \mathfrak{B}(\mathcal{H})$. A state ρ in a Hilbert space $\mathcal{H}$ then naturally gives rise to the algebraic state $\omega(A) = Tr(\rho\pi(A))$ for all $A \in \mathcal{A}$. And the GNS construction (named after Gel'fand, Naimark and Segal) allows us to move in the opposite

[23]In a little more detail: a C^* algebra is an algebra $\mathcal{A}$ over the field $\mathbb{C}$ of complex numbers, with an involution and a norm. The involution * satisfies: $(A^*)^* = A, (A+B)^* = A^* + B^*, (\lambda A)^* = \lambda^* A^*$ and $(AB)^* = B^* A^*$ for all $A, B \in \mathcal{A}$ and all $\lambda \in \mathbb{C}$ and where λ^* denotes the complex conjugate. Calling an element self-adjoint means that $A^* = A$. The norm, satisfies $||A^*A|| = ||A||^2$ and $||AB|| \leq ||A||||B||$. Clifton and Halvorson (2001, §) provides a philosophically oriented exposition and discussion.

[24]For an explanation and justification of the restriction to *bounded* observables, i.e., those associated with the bounded self-adjoint operators in $\mathcal{H}$, see Sewell (1986, 13-15).

direction. For any algebraic state ω in $\mathcal{A}$, there is a representation and a Hilbert Space, $(\pi_\omega, \mathcal{H}_\omega)$ of $\mathcal{A}$, together with a cyclic[25] vector $|\Psi_\omega\rangle \in \mathcal{H}_\omega$, such that $\omega(A) = \langle\Psi_\omega|\, \pi_\omega(A)\, |\Psi_\omega\rangle$ for all $A \in \mathcal{A}$. The GNS construction guarantees that for every abstract algebraic state there is a Hilbert space representation, and also guarantees that it is unique (up to unitary equivalence). Although we discussed this algebra as having arisen from a previously given Hilbert space theory, we are quite free to consider it in abstraction — as a theory in its own right, without any Hilbert space underpinnings.

For finite systems, the Hilbert space and Algebraic approaches co-exist peacefully, for the Stone-von Neumann theorem assures us that any two irreducible[26] representations of CCRs associated with a finite dimensional configuration space, will be *unitarily equivalent*. This means that for any two Hilbert space representations $(\mathcal{H}, \{\hat{O}_i\})$, and $(\mathcal{H}', \{\hat{O}'_i\})$, there exists a unitary map $U : \mathcal{H} \to \mathcal{H}'$ such that $U^{-1}O'_iU = O_i$ for all O_i. Unitary equivalence is generally interpreted as implying the equivalence of Hilbert space theories (in the sense that the two theories will deliver the same expectation values for corresponding observables; for further discussion on the link between unitary and physical equivalence, see Clifton and Halvorson (2001, §2.2-2.3)). However, for infinite systems, the Stone-von Neumann theorem does not hold, and in general there exist unitarily *in*equivalent representations of the CCR's. Yet the associated Weyl algebra is well-defined, and representation independent. The question immediately occurs: are the differences between unitarily inequivalent Hilbert space representations imbued with any physical significance? Or are they merely alternative formulations of the same physical theory?

[25]Cyclic means that $\pi_\omega(\mathcal{A})\, |\Psi_\omega\rangle$ is dense in $\mathcal{H}_\omega$. All representations can be expressed as direct sums of cyclic representations.

[26]A representation of $\mathcal{H}$ is *irreducible*, iff there are no non-trivial subspaces of $\mathcal{H}$ that remain invariant under the action of all operators in the representation.

Ruetsche sets up two extreme interpretative positions. The 'Hilbert space chauvinist' believes that the Hilbert Space approach is fundamental, and as such we have to choose a privileged representation as physical: all alternative representations are judged to be superfluous. In opposition, the 'algebraic chauvinist' treats the self-adjoint elements of the Weyl algebra as fundamental, and any distinctions amongst particular Hilbert space representations are distinctions without a physical difference.

An adherent to either of these extreme positions soon meets difficulties when they try to interpret quantum field theories. The algebraic chauvinist cannot admit many unbounded operators that we would like to invest with physical significance, since they only appear in a particular representation (e.g., position, momentum and the number operator). The Hilbert space chauvinist is forced to choose a particular representation and to deny that any states not in this privileged Hilbert space possess physical significance. Each of Ruetsche's two positions are extreme, and might well be said to play the roles of straw-men (though she presents them as realistic, and associates her algebraic chavinist with quotes from Segal). But the continued debates in the interpretation of field theories demonstrate the difficulty of defining the best intermediate position — see for example: Ruetsche (2002), Clifton and Halvorson (2001), Kronz and Lupher (2005).

5.2 QSM and the Thermodynamic Limit

Ruetsche looks to quantum statistical mechanics for guidance on her interpretative position. She notes that neither chauvinist can accommodate the representational work that unitarily inequivalent representations do within QSM, at least once we demand that such a statistical theory must accommodate phase transitions. For as in the classical case, in quantum statistical mechanics we need to take the thermodynamic limit before it is possible to model phase transitions. And there the unitarily inequivalent representations *do* attain a very firm physical significance. We should look briefly at how this arises.

Let us consider a QSM system (finite or infinite) as modelled in the C^* algebraic framework. The system can be represented by the pair $(\mathcal{A}, \alpha_t)$: a C^* algebra $\mathcal{A}$, and a one parameter group of automorphisms α_t, which for all states $A \in \mathcal{A}$, represents their evolution through a time t. Let the system have inverse temperature $\beta = \frac{1}{kT}$. Now consider an algebraic state ω which satisfies the following condition:

$$\omega\left[A\alpha_{i\beta}(B)\right] = \omega(BA) \text{ for all } A, B \in \mathcal{A} \tag{6}$$

We say that a state satisfying this condition is a KMS state with respect to the automorphism group α_t at inverse temperature β.[27] For a finite system this KMS state exists, and is unique. And when the state is given a particular Hilbert space representation, by the correspondence scheme described above, it matches that given by the usual density matrix of Hilbert space Gibbsian statistical mechanics, viz,

$$\hat{\rho} = \frac{e^{-\beta\hat{H}}}{Tr\left[e^{-\beta\hat{H}}\right]} \tag{7}$$

(where again $\beta = \frac{1}{kT}$, and the dynamics will be given by the family $\hat{U}_t = e^{-i\hat{H}t}$ of unitary operators generated by the Hamiltonian $\hat{H}$). The Gibbs state is the unique Hilbert space state associated with the thermodynamically stable state of a quantum system with the Hamiltonian $\hat{H}$, so this encourages us to identify the KMS state as the algebraic version of a thermodynamically stable state. But when

[27]The states are named after Kubo, Martin and Schwinger who first pointed out the thermodynamic properties of states satisfying Equation 6. (Being a little more careful, we say that KMS states must satisfy the condition in a dense subalgebra of $\mathcal{A}$.) For more discussion and a precise formulation see, for example Emch (2006, §10.4), which also gives details of the rich stability properties of KMS states.

we want a theory of phase transitions, the uniqueness of the equilibrium state for each temperature becomes a curse.

One way to get away from the uniqueness is to consider the TD limit, but now the picture starts to break down, for the Gibbs state of Equation 7 is not well-defined for infinite systems. Fortunately KMS states are more general, and we can find states of infinite systems that satisfy Equation 6. And it is possible to motivate the identification of these KMS states with thermodynamic equilibrium states, even without the motivation of a corresponding Gibbs state. For example, where KMS states are unique, they satisfy both local and global thermodynamic stability conditions against perturbations of state, including invariance under the dynamical group α_t (Sewell (2002, 113-123) and Emch (2006, §10.4)). It is also a theorem that if there is a unique (α_t, β)-KMS state, then that state is a *factor state*, and these are characterised by features such as a lack of long-range correlations and fluctuations, leading us to identify them with pure thermodynamic phases. (There is more motivation for this identification; Sewell (1986, §4.4)).

But in the infinite limit, we can also find automorphism groups α_t and inverse temperatures β such that there are a plurality of (α_t, β)-KMS states. But each algebraic state ω in this plurality can be decomposed uniquely into extremal KMS states (Emch and Liu, 2005, 158-160). Let us suppose that there are two such: ω_1 and ω_2. Besides, these extremal states can be shown to be pairwise *disjoint*, which means that no algebraic state that we can express as a density matrix on Hilbert space representation $(\mathcal{H}_{\omega_1}, \pi_{\omega_1})$ can be expressed as a density matrix on $(\mathcal{H}_{\omega_2}, \pi_{\omega_2})$. In other words, the unique decomposition gives us extremal states that are not representable in the same Hilbert Space, for they live in unitarily inequivalent representations. And these extremal states are again factor states, which we have seen are associated with pure thermodynamic phases.

We are led to the following picture: QSM represents states of thermodynamic phase by KMS states. In finite systems, these are always unique and correspond to the Gibbs state, but in infinite systems they are not unique. But they can be decomposed into extremal, factor states, which can only be represented in unitarily inequivalent Hilbert spaces. One final piece of information is needed to complete the picture: the algebraic framework represents temperature as a "global" superselected observable, which is a constant number for each representation.

Ruetsche points out that both chauvinists are in trouble. For the difference between inequivalent representations is the only aspect that distinguishes the different states. The algebraic chauvinist is committed to consider such a distinction unphysical, since it is not represented in their semi-local algebra. On the other hand, the Hilbert space chauvinist is meant to select a single representation, and consider all others to be unphysical. And this would commit them to holding that only one equilibrium state was physically possible with only one temperature, and so lose their theory of phase transitions.

5.3 Lessons Applied

Considering these and similar problems Ruetsche is led to advocate "grades of physical possibility". One thinks of the algebraic states as picking out the broadest sort of possibility: the totality of states available to a given system. Then, by choosing a particular Hilbert space representation we narrow down possibility, fixing physical contingencies such as temperature and representing only those states consistent with them. Ruetsche (2003, 1339-41) admits that her approach is only a sketch of a position, and grants that the idea of 'treating physical possibility as a matter of degree' is one that needs to be developed in more detail.

Since Ruetsche's position is at present only an outline, it is hard to estimate its promise. But I am concerned by her belief that if the position can be filled out it can be hoped to provide a general understanding of quantum theories with infinite degrees of freedom (ibid, 1341). For it appears to me that she has drawn general lessons about representational significance from just those features which are bound up with peculiarities specific to the TD limit.

This can be seen if we repeat the question of why we take the TD limit, but this time for quantum rather than classical statistical mechanics. Again, the statistical theory is intended to model a finite system, but we appeal to the TD limit nonetheless. Of the three motivations separated in §2.3, let us ignore the consideration of mathematical convenience, for the algebraic approach is fairly difficult to use for everyday calculations in any case. And at the level of generality we are considering, the motivation of seclusion is less important, for we could run the same discussion with a very "clean" example of a single type of phase transition, which needs no further isolation.

We are left with our motivation for taking the TD limit, as providing the theory with enough *structure* to provide a satisfactory theory of phase transitions. And this can be identified with the fact that it is only in the TD limit that the KMS state can become non-unique and non-trivially decomposable into extremal states — exactly the structure needed to provide a theory of phase transitions.

The clearest way of appropriating this structure requires us to recognise physical significance in the unitarily inequivalent representations of states. But then Ruetsche's point that neither of her 'chauvinists' are able interpret the new structure in a straightforward manner, is hardly surprising. As we have just seen, it is also difficult to interpret the structure provided by the TD limit in the classical case. But this suggests that both the Hilbert Space chauvinist and the Algebriac chauvinist can follow the lead of the classical discussion, and make use of the newly available mathematical structure, without compromising their position. Let us briefly sketch how this can be done.

First, the Hilbert Space chauvinist can consider the KMS/Gibbs equilibrium state to provide the most direct representation of any finite system. But to analyse phase transitions, he must consider the TD limit, in particular he must ask whether the KMS state in that limit is unique and extremal. He can hold that it is facts about the original finite KMS/Gibbs state that determines how the infinite KMS state should be constructed; and thus it is the finite system state that determines the nature of any infinite system states, which describe phase transitions. The fact that he cannot consider more than one representation of this infinite KMS state as directly representational becomes irrelevant — he does not need to.

The Algebraic chauvinist is equally free to consider the finite KMS/Gibbs state as the directly representational one (though he will feel that it is the KMS algebraic state that is primary, as opposed to its particular Hilbert space representation as a Gibbs state). And when he looks to the infinite KMS state in the TD limit, he is not limited to the semi-local algebra when he looks for a temperature observable. The GNS construction gives him the structure he needs to distinguish temperatures, and he can hold that this construction is encoded in the original (finite) algebraic state, even if it did require a diversion through the infinite limit, and through the structure of inequivalent Hilbert space representations to use it.

We can see that both Ruetsche's original problem (the inadequacies of the resources available to the chauvinists), and its solution (as outlined above) arise directly due to the pecularities of the representational role of the TD limit, in exact parallel with the classical cases. So Ruetsche's suggestion that we should take interpretative lessons across to a situation in which the infinite nature of the system is to be interpreted realistically — such as a field theory — appears at least questionable.

At the end of her article, Ruetsche briefly considers the objection that she may 'have rested interpretative conclusions on the consideration of a setting which is a hotbed of manifest falsehoods and extreme idealisations' (Ruetsche, 2003, 1342).

Her response is simply to deny the charge, holding that her interpretative conclusions are resting on 'those facets of the thermodynamic limit that appear to do representational work'; a contention she supports by pointing out their indispensibility to the structure of the theory. My response should be clear: while the TD limit is indeed indispensible, this does not mean it plays a direct representational role, and certainly not that we should draw on it to inform wide-ranging interpretative doctrine.

For vividness, we can push the parallel with the classical case a little further. Imagine that we looked at a classical field theory such as electromagnetism, and wondered how to interpret any non-analyticities in the fields. The analogue of Ruetsche's argument would be to look to the TD limit of classical statistical mechanics, note that it made a central and ineliminable use of non-analyticities to represent an element of physical reality, and argue that electromagnetism must admit them as well.[28] Using this classical statistical mechanics to guide our interpretation of a classical field theory would — I suggest — be as misguided as using quantum statistical mechanics to guide our interpretation of quantum field theory.

5.3.1 Effective Field Theories

All this having been said, there is an oft-discussed interpretative position, within which QSM *would* be relevant to the interpretation of unitary inequivalence. One contemporary approach to understanding many of the pecularities of QFTs, such as the existence of infra-red and ultra-violet divergences, and their renormalisability, is that they should be understood as "effective" field theories. That is, they are to be understood as valid only for a particular energy scale, absorbing

[28]It might be objected that the representational role of the free energy function in statistical mechanics is not sufficiently analogous to that of the electromagnetic field. A closer parallel would be to the order parameter field. This is defined over space-time points, and will have singularities at many varieties of phase transition.

the effects of small-scale/high-energy interactions into the definition of the field parameters. In particular, there have been suggestions that the understanding of renormalisation techniques as applied to phase transitions in condensed matter physics, show that renormalisability is a "signature" of an effective field theory. So the renormalisability of present field theories should make us hesitate to interpret them as directly representing any fundamental furniture of the world.

I discuss this view of quantum field theories in Mainwood (2006, Chap. 5), but it bears on Ruetsche's thesis. For if we accept the "effective field" view, with an added hypothesis that the unknown higher-level theory is one with a finite dimensional state space, then lessons from the interpretation of QSM start to look a great deal more relevant. Objects such as the order-parameter field would be seen as a variety of effective field, in that they summarise the effects of many lattice interactions into a continuous field. And this treatment also breaks down at certain energy scales (i.e., those that probe distances comparable to the lattice spacing). In this way we might consider the infinite nature of QFTs as having arisen in a way analogous to the TD limit. But there are at least two extremely controversial presuppositions that would have to be made before adopting this position. First, we would have to hold that all present quantum field theories are effective; second, that the higher energy theory, of which they are merely a low-energy limit, is a discrete theory with finite degrees of freedom. If Ruetsche is committed to both of these theses she does not give any hint of it. In contrast, she writes throughout as though she wants to interpret quantum field theories as straightforward a manner as possible, directly describing fundamental features of the world.

6 Concluding Remarks

We have arrived at the following picture. Only in the infinite limit can we find the mathematical apparatus used to describe and categorise phase transitions. The density of zeroes in the complex plane (Lee-Yang), the orders of discontinuities in the free energy (Ehrenfest and modern variants), and the nature of the fixed points (renormalisation), all give a fruitful analysis of different types of phase transitions. On the other hand, the phase transitions that are actually observed and against which these theories are tested take place in systems that appear to be finite.

The natural position would be one that endorses the indispensability of the TD limit for our successful theories of phase transitions, but without denying the evident fact that they occur in the finite systems we see around us. The definition in §4.1 is a proposal that allows us to occupy exactly such a position, allowing us to define the finite instances as fully genuine phase transitions (albeit sometimes "messy" or "hybrid" examples).

Naturally, the proposal offered is not the only way in which we can occupy such a position. But I feel that it must be occupied in some way, for the alternatives are untenable. To argue that it is only for the sake of simplicity in our mathematics that we cling to the infinite limit is to fail to recognise that it makes available a taxonomy and structure which are essential to an adequate theory of phase transitions. And if we admit its indispensibility, but try to deny that finite systems exhibit "true" phase transitions, then we face a dilemma. Either we hold that all empirical phenomena are in fact aspects of infinite systems, or we hold that the phenomena represented by the theory are not those empirical phenomena we observe. If we take the first option then we are committed to the view that we have evidence of the infinite nature of physical systems every time we see a kettle boil. But taking the second option is to hold that our most successful theories cannot be applied to the phase transitions we test them against. Unless we can provide a coherent story of how our infinite theories can acquire empirical significance nonetheless, their success becomes a mystery.

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