What Is the Paradox of Phase Transitions?

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I present a novel approach to the scholarly debate that has arisen with respect to the philosophical import one should infer from scientific accounts of phase transitions by appealing to a distinction between representation understood as denotation, and faithful representation understood as a type of guide to ontology. It is argued that the entire debate is misguided, for it stems from a pseudo-paradox that does not license the type of claims made by scholars and that what is really interesting about phase transitions is the manner by which they force us to rethink issues regarding scientific representation, idealizations, and realism.

1. Introduction. Phase transitions (PT) include a wide variety of common and not so common phenomena in which the qualitative macroscopic properties of a system or a substance change abruptly. Such phenomena include, among others, water freezing into ice or boiling into air, iron magnetizing, graphite spontaneously converting into diamond, and a semiconductor transitioning into a superconductor. There exists a flourishing scholarly debate with respect to the philosophical import one should infer from the scientific accounts of phase transitions, in particular, the accounts' appeal to the thermodynamic limit (TDL), and regarding how the nature of PT is best understood. It has become standard practice to quote the authoritative physicist Leo P. Kadanoff, who is responsible for much of the advances in renormalization group methods and in understanding PT, in order to better illustrate the puzzlement associated with PT: "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). If we add to the above that observations of boiling kettles confirm that finite systems do

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undergo PT, we conclude that a rather odd paradox arises: PT do and do not occur in finite, and thus concrete and physical, systems. The above is taken as a basis for warranting such scholarly claims to the effect that PT are irreducible emergent phenomena (e.g., Prigogine 1997, 45; Lebowitz 1999, S346; Liu 1999, S92; Morrison 2012, 143), which necessitate the development of new physical theory (Callender 2001, 550), and for inducing a wide array of literature that argues to the contrary (e.g., Batterman 2005; Bangu 2009; Wayne 2009; Butterfield 2011; Norton 2012; Menon and Callender 2013).

In this article, I would like to build on the works of Mainwood (2006) and Jones (2006) to further investigate what exactly is the paradox of PT, which is meant to license the type of scholarly conclusions and discussions noted above. It seems to me that a natural condition of adequacy for the particular claim that PT are emergent phenomena, as well as the more general debate that arises, is that there really is a bona fide paradox associated with PT. In other words, it really must be the case that a phase transition "is emergent precisely because it is a property of finite systems and yet only reducible to micro-properties of infinite systems" (Liu 1999, S104) or, more recently, that "the phenomenon of a phase transition, as described by classic thermodynamics cannot be derived unless one assumes that the system under study is infinite" (Bangu 2009, 488). Accordingly, in section 2, I describe the paradox and suggest that much of the debate revolving around PT stems from it. In doing so, I appeal to Contessa's (2007, 52–55) distinction between representation understood as denotation, and faithful representation understood as a type of guide to ontology (Sklar 2003, 427). Afterward, I will continue to argue for a negative and a positive thesis. My negative thesis is that there really is no paradox of phase transitions and that in order to get a bona fide paradox, that is, a contradiction, one must undertake substantial philosophical work and ground a type of indispensability argument, akin to the kind appearing within the context of the philosophy of mathematics. Since none of the proponents of the PT debate undertake such work, and since indispensability arguments are highly controversial, I claim that the entirety of the debate, insofar as it is grounded in the paradox of PT, is misguided and that the philosophical import that has been extracted from the case study of PT with regard to emergence, reduction, explanation, and so on is not warranted.

However, I also have a positive thesis. In section 2.1, I show how the paradox can be generalized and arises whenever a scientific account appeals to an essential idealization (EI)[1]—roughly, when a scientific account of some concrete physical phenomena appeals to an idealization in which, in principle, one cannot attain a more successful account of said phenomena by "de-

1. Butterfield (2011) and Mainwood (2006) use the term "indispensible," Jones (2006) uses "ineliminable," and Batterman (2005, 2013) uses "essential."

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idealizing" the idealization and producing a more realistic idealization. In doing so, I suggest in section 3 that what is really interesting about phase transitions is the manner by which they illustrate the essential idealization problem (EIP), which is tightly connected to issues arising in the context of scientific representation and scientific realism. The upshot is that, insofar as proponents of the phase transition debate have been contributing to the EIP, certain aspects of the debate have been fruitful. Consequently, I outline various possible solutions to the EIP and the paradox of PT, which have been extracted from Butterfield (2011) and Norton (2012). I suggest that, although such solutions pave the road for further work to be done, it is questionable whether they are conclusive and exhaustive.

2. What Is the Paradox of Phase Transitions? In his 2001 paper "Taking Thermodynamics Too Seriously," Craig Callender presents several allegedly true propositions that jointly induce a paradox concerning PT—that concrete systems can and cannot undergo PT:[2]

1. Concrete systems are composed of finitely many particles N.
2. Concrete systems display PT.
3. PT occur if and only if the partition function Z has a discontinuity.
4. The partition function Z of a system with finitely many particles N can only display a discontinuity by appealing to the TDL.
5. A system in the TDL has infinitely many particles.[3]

Tenets 1–2 imply that concrete and finite systems display phase transitions while tenets 3–5 imply that only infinite systems can undergo phase transitions. However, contra Bangu (2009), Callender (2001), Mainwood (2006), Jones (2006), and others, I contend that no contradiction arises by conjoining tenets 1–5. To see this, we must first distinguish between concrete PT, on the one hand, and abstract mathematical representations of them, on the other hand.[4] To be clear, a "concrete" system would include a physical thermal system of the type we find in the world or in a lab, while "abstract mathematical" just refers to pieces of math, for example, a set with a function

2. The paradox of PT presented here is not the exact version presented in Callender (2001, 549). Instead, I present the paradox in a manner that is more relevant to my discussion. Several authors, such as Mainwood (2006, 223) and Jones (2006, 114–17), have undertaken a similar approach.

3. For precise characterization of various forms of the TDL, see Norton (2012, secs. 3 and 4) and reference therein.

4. The distinction between concrete and abstract objects is well known. Abstract objects differ from concrete ones in the sense that they are nonspatiotemporal and causally inefficacious. Paradigm examples include mathematical objects and universals. Compare Rosen (2001).

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defined on it. Also, I take the term "representation" here to be stipulated denotation that is agreed upon by convention.[5] For instance, the notation "N" represents "the number of particles" (in a given system) in the sense that it denotes the number of particles. Second, notice that there are ambiguities with regard to whether the terms "PT" and "partition function" ("Z") in tenets 3 and 4 refer to concrete objects or abstract mathematical representations of them. As concrete objects, PT are concrete phenomena or processes that arise within concrete systems, while Z is some sort of concrete property of such systems. As abstract mathematical representations, both PT and Z are just pieces of mathematics that allegedly denote concrete objects. To avoid confusion, note that by "abstract PT" I only mean PT in the sense that an abstract Z displays a discontinuity. In the same manner, there is a clear ambiguity concerning the physical interpretation, that is, the concreteness or abstractness, of the TDL.

Thus, for example, if "PT" and "Z" in tenets 3 and 4 refer to abstract mathematical representations, as opposed to concrete objects, then there is no paradox: concrete and finite systems display PT while abstract and finite ones do not. Just because abstract mathematical representations of concrete systems with finite N do not display PT does not mean that concrete finite systems do not display PT. Alternatively, if "PT" in tenets 3 and 4 do refer to concrete PT, it also does not immediately follow that there is a paradox. Rather, what follows is that concrete PT occur when abstract representations of them display various abstract properties, such as a discontinuity in Z and an appeal to the TDL. One might wonder what explains this particular correlation between discontinuities in abstract representational partition function and concrete phase transitions. However, prima facie, there is no paradox.

The point is that without adding additional tenets that make a claim about the relation between, on the one hand, concrete PT occurring in physical systems and, on the other hand, the abstract mathematical representation of concrete PT, which arise in scientific accounts of PT, no paradox arises. In the following subsection, I will add such additional tenets in hope to further shed light on the central philosophical issue that arises in the context of PT. To end, it is worth noting that, if my claim about there being no paradox is sound, then the entire debate revolving around PT, insofar as it is grounded in the paradox of PT as stated above, is unmotivated and misguided. In particular, notice that the various positions expressed with regard to the debate can be delineated by identifying which tenet of the paradox a particular proponent denies or embraces. Authors such as Lebowitz (1999, S346), Liu (1999, S92), Morrison (2012, 143), and Prigogine (1997, 45) can be read as embracing tenet 3 and identifying PT as a kind of nonreductive emer-

5. Compare Contessa (2007, 52–55) and references therein.

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gent phenomena. Contrasting attitudes have been voiced by Wayne (2009), where Callender (2001) and Menon and Callender (2013) explicitly deny that phase transitions are irreducible and emergent phenomena by rejecting tenet 3. Butterfield (2011) can be read as both denying and embracing tenet 3, in an effort to reconcile reduction and emergence. Norton (2012) can be understood as denying tenet 5. I refer the reader to Mainwood (2006, 223–37), who presents an exposition of this type of delineation—that is, a classification of scholarly attitudes to the nature of phase transition grounded in the paradox. For my purposes, what is important is to identify that the large majority, if not all, of the phase transition debate arises from the phase transition paradox.

2.1. The Bona Fide Paradox of Phase Transitions and Its Generalization. The key ingredient necessary to engender a bona fide paradox is for a particular kind of correspondence relation to hold between abstract representations and concrete systems. To make this point clear, we must appeal to a further distinction. While I take "representation" to be stipulated denotation, by "faithful representation" I mean a representation that allows agents to perform sound inferences from the representational vehicle to the target of representation (Contessa 2007, 52–55). That is to say, a faithful representation allows agents to make inferences about the nature of the target of representation. Thus, it acts as a kind of guide to ontology,[6] since it accurately describes aspects of the target of representation. In other words, a faithful representation is one in which the vehicle and target of representation resemble each other in some manner, for example, they share some of the same, or approximately same, properties and/or relations. The classic example here is a city map, which is a faithful representation of a city because it allows us to perform sound inferences from the vehicle to the target, that is, from the map to the city. This is so because both the vehicle and the target share various properties. For instance, if two streets intersect in the map, then they also intersect in the city. That is to say, intersecting streets in the map correspond to intersecting streets in the city. Therefore, the map acts as a type of ontological guide that accurately describes the city. For instance, there *really* are intersecting streets in the city. It is worth noting that my account potentially differs from Contessa (2007), who isn't clear about the ontological aspect of faithful representations. Contessa (2007) differentiates from "epistemic representation," from which valid inferences can be drawn, and faithful ones that permit sound inferences. Whether or not such inferences come with ontological baggage depends on whether they are about the target itself. On my account, faithful representations license sound inferences about the target itself, and hence they the fix the ontology of the target.

6. Compare Sklar (2003, 425).

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With this distinction in hand, if we add a tenet that states that the abstract representational discontinuities representing phase transitions are faithful and hence correspond to concrete physical discontinuities, we do get a genuine contradiction. This is so because if systems are composed of finitely many particles, which is the case within the context of the atomistic theory of matter conveyed in tenet 2, then it makes no sense to talk of concrete discontinuities. The notion of concrete discontinuities presupposes that matter is a continuum so that there can be an actual discontinuity. Otherwise, an apparent discontinuity is actually the rapid coming apart of particles and not a real discontinuity. Consequently, adding a tenet as the one just described amounts to claiming that systems are not composed of finitely many particles, and so we get: concrete systems are and are not composed of finitely many particles N.

In a similar manner, one can engender a kind of paradox by reifying the TDL through an appropriate correspondence relation. For instance, one could add the tenet that an appeal to the TDL, which could be interpreted as a type of continuum limit faithfully representing an abstract system, in fact faithfully represents a concrete system. Thus, we deduce the claim that concrete systems are and are not composed of finitely many particles N (in the sense that the ontology of concrete systems is both atomistic and that of a continuum, i.e., not atomistic).

The source of the problem of PT seems to be that the mathematical structure that scientifically represents concrete PT—a discontinuity in the partition function—is an artifact of an idealization (or an approximation), the TDL, which is essential in the sense that when one "de-idealizes" said idealization, the mathematical structure representing PT no longer exists.[7] Accordingly, I would like to suggest that what is really interesting about PT is the manner by which they might shed light on the nature of scientific representation and idealization. In particular, notice that once concerns regarding representations are incorporated, the paradox of PT can be generalized by making use of the concept of an EI:

1. Concrete systems include a concrete attribute A.
2. Concrete systems display a concrete phenomenon P.
3. P is scientifically-mathematically represented by P'.
4. P' can only arise by appealing to an idealizing limit I.
5. A system in the idealizing limit I includes an attribute $A^{\approx}$ such that $A \neq A^{\approx}$.
6. P' faithfully represents P.

7. For a more precise statement to this effect, see Butterfield's (2011, 1123–30) and Mainwood's (2006, 216–18) discussion of Yang-Lee theory and Kubo-Martin-Schwinger states.

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Tenets 1 and 2 imply that concrete systems are A and display P. Tenets 3–5 imply that P is scientifically represented by P', which presupposes $A^{\approx}$. Tenet 4 encompasses our EI since any de-idealization of I will render P' nonexistent. So far there is no contradiction. But, when one adds the correspondence relation described by tenet 6, a bona fide paradox arises: concrete systems are and are not A (since they are A and they are $A^{\approx}$, and $A \neq A^{\approx}$). What is important to notice is that tenets 1 and 2 are claims about concrete systems, wherein tenet 2 identifies the concrete phenomenon to be scientifically accounted for, while tenets 3–5 are claims about abstract scientific accounts of concrete systems, and it is tenet 6 that connects the abstract with the concrete via faithful representation, thereby engendering a genuine paradox. The question, of course, is why would one endorse tenet 6? The answer is that without tenet 6 the entire scientific account of the concrete phenomenon in question seems somewhat mysterious to anyone with noninstrumental sympathies. In particular, those with realist intuitions will want to unveil the mystery with a correspondence relation that tells us that our abstract scientific accounts get something right about the concrete world. But how would one argue for a correspondence relation along the lines of 6? It seems to me that, given the "essentialness" aspect of the idealizing limit that arises in tenets 3 and 4, the only way to justify tenet 6 is by appeal to an indispensability argument.[8] In other words, something of the sort:

1. A scientific account of some concrete phenomena appeals to an idealization(s) and refers to idealized abstract objects.
2. The idealization appealed to is essential to the scientific account in the sense that any de-idealization renders the scientific account less successful and the idealized abstract object nonexistent.
3. Hence, the idealization appealed to, and the idealized abstract objects made use of, are indispensable to the account.
4. Thus, as scientific realists, we ought to believe that such abstract idealized objects do exist. Further, the ontological import of such idealizations is true of concrete systems, on pain of holding a double standard.

Said differently, and in the specific cases of PT, since reference to a discontinuity in Z is indispensable to scientific accounts of PT, and since these discontinuities only arise by appealing to EI, we ought to believe in the existence of concrete discontinuities.

8. For a survey of the indispensability argument of mathematics and a defense, see Colyvan (2001).

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Thus, in contrast to many of the scholars engaged in the phase transition debate, who assume that there is a paradox and then continue to attempt to dissolve it by some manner or other, I claim that in order to get a genuine paradox, one needs to justify a correspondence relation (such as the one appearing in tenet 6) by appealing to an indispensability-type argument. Since cogent indispensability-type arguments require serious philosophical work and are very much controversial, and since no author engaged in the phase transition debate has undertaken such work, it follows that much of the controversy revolving around phase transitions is not well motivated. That is to say, claims to the effect (i) that PT are or are not emergent, (ii) that they are or are not reducible to statistical mechanics (SM), and (iii) that they do or do not refute the atomic theory of matter are grounded in a frail foundation that does not license such significant conclusions.

One might worry that, contrary to my claims, a bona fide paradox of PT can arise on the epistemological level by conceding to a set of tenets from which it is possible to deduce that SM does and does not govern phase transitions. The idea here is to argue that "SM-proper" is not licensed to appeal to the TDL and so SM-proper does not govern PT. However, the objection continues, it is generally assumed that SM is the fundamental theory that governs PT. Thus, we have a paradox, and the natural manner by which to dissolve it is to argue that SM-proper does indeed have the tools to account for PT (Callender 2001; Menon and Callender 2013), or else to claim that PT are emergent. In reply, it is far from clear to me that SM-proper is not licensed to appeal to the TDL, and so that it does not govern PT. In fact, there are reasons to think that the TDL is part and parcel of SM-proper because (*a*) it is common practice to appeal to the TDL in modern approaches to SM, and (*b*) the TDL is used in SM not only to account for phase transitions but to account for, among others, the equivalence of SM ensembles, the extensivity of extensive thermodynamic parameters, Bose condensation, and so on (Styer 2004). In addition, (*c*) all the best scientific accounts of PT, and these include mean field theories, Landau's approach, Yang-Lee theory, and renormalization group methods, represent PT as discontinuities by appealing to the TDL, and (*d*) the large majority of empirically confirmed predictions of SM, within the context of PT and beyond, appeal to the TDL.

Moreover, even if it were the case that SM-proper is not licensed to appeal to the TDL, no contradiction would arise. Rather, it would be a brute fact that SM-proper does not govern phase transitions and "SM-with-the-TDL" does. If then it is claimed that the ontologies of SM-proper and SM-with-the-TDL are radically different so that indeed there is a paradox, we must notice that such a claim amounts to no more than reviving the paradox at the level of ontology, and hence my discussion in this section bears negatively on this claim.

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Finally, the claim that PT are emergent because SM-proper cannot account for them seems to replace one problem (i.e., PT are not governed by the fundamental theory) with another problem (i.e., PT are emergent). How does dubbing PT "emergent" illuminate our understanding of them or of their scientific accounts? How is this philosophically insightful? Accordingly, I endorse Butterfield's (2011) description of emergence as novel and robust behavior, as opposed to a failure of intertheoretic reduction of some sort.

3. The Essential Idealization Problem. The above discussion points to what I consider to be the central philosophical issues arising out of the debate concerning PT. First, the discussion regarding (i) the need for a correspondence relation between our abstract scientific-mathematical representations and concrete systems, (ii) the appeal to the concept of "faithful representation," and (iii) the identification that the phase transition paradox can be generalized to any scientific account that appeals to EI, demonstrates that a solution to the following problem is needed:

> **The Essential Idealization Problem** (**EIP**)**.** We need an account of how our abstract and essentially idealized scientific representations correspond to the concrete systems observed in the world, we need a characterization of EI, and a justification for appealing to EIs, i.e., an explanation of why and which EIs are successful, which does not constitute a de-idealization scheme.[9]

To this effect, Batterman (2005, 2010, 2013) has made progress by explaining that it is not at all clear that traditional mapping accounts of scientific and mathematical representation work in cases of EI. In particular, this is so because the abstract mathematical structure doing the representational work does not "latch on," and so is not partially isomorphic or homomorphic, to any concrete physical structures in the external word. Moreover, insofar as the physical world constrains scientific representations, there are reasons to think that consideration of scale size, in which the phenomenon of concern occurs, plays an important role in modeling and scientifically representing such phenomena.

Second, the discussion of indispensability makes it clear that the mystery revolving around the EIP is truly mysterious for those with scientific realist sympathies and, in fact, may threaten certain conceptions of realism. This follows because, insofar as arguments like the "no miracles argument" and

9. Mainwood (2006, 214–15) also identifies a similar problem but in a context that is different from mine, and his solution (238), endorsed by Butterfield (2011), misses the central issue discussed here.

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"inference to best explanation" are cogent and give us good reason to believe the assertions of our best scientific accounts, including those about fundamental laws and unobservable entities, then in the case of accounts appealing to EI, these arguments can be used via an indispensability argument to reduce the realist position to absurdity. What is needed is a realist characterization of EI and solution to the EIP, and thus a realist account of PT.

In fact, such potential solutions to the paradox of PT can be extracted from two recent contributions to the debate: Butterfield (2011) and Norton (2012). Although it is beyond the scope of this article to treat these contributions thoroughly, I will end by discussing them shortly in an effort to support my suggestion that, although such solutions pave the road for further work to be done, it is questionable whether they are conclusive and exhaustive.

Butterfield (2011) grants that the TDL is "epistemically indispensable" for the emergence of the novel and robust mathematical structure that is used to represent PT, but denies that any paradox emerges because the limit is not "physically real." Using the terminology expressed here, the discontinuities in Z play a representational role but not a faithfully representational one. The question arises, how come unfaithful representations work so well? To that end, Butterfield (2011, sec. 3) appeals to the distinction, also used by Norton (2012, sec. 3), between "limit quantities" or "limit properties," that is, the limits of properties, and a "limit system," that is, the system at the limit. He continues to argue that the behavior of certain observable properties of concrete finite systems, for example, magnetization of a ferromagnet, smoothly approaches the behavior of the corresponding properties of abstract infinite systems. Moreover, it is the large N behavior, not the infinite N, which is physically real.

Norton (2012) suggests that by viewing the TDL as an approximation—an inexact description of a target system, instead of an idealization—a novel system whose properties provide inexact descriptions of a target system, we can diffuse any problems that might arise. Within the context of our discussion, Norton's idea is that no paradox can arise if the TDL is an approximation, since approximations do not refer to novel systems whose ontology might be drastically different from the target system's ontology, thereby engendering a paradox once we add an appropriate correspondence relation. In a manner similar to Butterfield (2011), his justification for appealing to such an approximation is pragmatic: the behavior of the nonanalytic Z belonging to an infinite system is approached by an analytic Z corresponding to a finite system with large N.

From my viewpoint, this cannot be the whole story. First, both accounts seem to ignore that it is a mathematical structure that arises only in the limit that is doing the representational work for us. Moreover, the accounts seem

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to suggest that we must revise our definition of PT as occurring if and only if the partition function has a discontinuity and substitute it with something along the lines of "PT occurs when various thermodynamic potentials portray sufficiently extreme gradients." The weakness of this suggestion is that we have substituted a precise characterization of PT with a vague one. But more problematic is the idea that we should be able to construct a finite N system that has, say, a Helmholtz free energy with an extreme gradient, which does not evolve into a discontinuity once the TDL is taken.[10] Second, the Butterfield-Norton approach outlined above seems incomplete, for it does not give us an account for why it is the case that the concrete external world constrains us to model and scientifically represent certain phenomena with mathematical structures that only emerge in some limit. For this purpose, talk of "mathematical convenience," "empirical adequacy," and "approximation" (understood as a purely formal procedure) misses what seems to be the truly intriguing features of PT. My suggestion is that we can further advance our understanding of PT, and similar phenomena that give rise to the EIP, by attempting to amend accounts like Butterfield's (2011) and Norton's (2012) with some of the key insights of Batterman (2005, 2013) regarding what mathematical techniques one must appeal to in order to properly represent certain kinds of phenomena. The details of this suggestion, as well as potential solutions to the EIP, are currently being developed and will be presented in future work.

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10. Mainwood (2006, 232) makes the same point.

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