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Diagrams as Part of Physical Theories: A Representational Conception

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Abstract. Throughout the history of the philosophy of science, theories have been linked to formulas as a privileged representational format. In this paper, following [8], I defend a semantic-representational conception of theories, where theories are identified with sets of scientific re-presentations by virtue of their epistemic potential and independently of their format. To show the potential of this proposal, I analyze as a case study the use of phase diagrams in statistical mechanics to convey in a semantically consistent and syntactically correct way theoretical principles such as Liouville's theorem. I conclude by defending this philosophical position as a tool to show the enormous representational richness underlying scientific practices.

Keywords: Phase diagrams · Semantic conception · Physical representations

1 Introduction

Throughout the history of the philosophy of science in the twentieth century, scientific theories have been constantly linked to sets of symbolic formulas (whether logical or mathematical) as the privileged representational format to convey their theoretical content or to reconstruct them rationally. Here I will defend the recent proposal of [8], who argue for a semantic-representational (in contrast to the semantic-structural) conception of scientific theories, where these are constitutively identified with sets of scientific representations by virtue of their capacity to provide scientific knowledge and independently of their format (i.e. formulaic, diagrammatic, iconic, etc.). To show the potential applicability of this philosophical proposal, we will analyze in detail as a case study the use of phase diagrams in statistical mechanics. From this analysis we will conclude that these phase diagrams could be satisfactorily understood as vehicles capable of conveying in a semantically consistent and syntactically correct way theoretical principles of statistical mechanics such as Liouville's theorem. We will conclude by defending this position as a tool to show the enormous representational richness underlying scientific practices.

2 Conceptions of Scientific Theories

During the twentieth and twenty-first century philosophy of science, scientific theories have been characterized in a variety of ways [4]. Initially, in logical positivism (whose

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history extends from the 1920s to the late 1950s) they employed the formal logical tools developed by Frege, Russell and Wittgenstein to characterize or 'rationally reconstruct' scientific theories as sets of symbolic formulas generated by means of axiomatically articulated logical languages. The logical architecture of scientific theories was determined 'syntactically' by a set of axioms expressed as primitive symbols, assigning empirical content by means of correspondence rules. In the context of this syntactic conception of theories, the relationship between diagrammatic vehicles (and of course also other non-syntactically defined iconographic elements) and scientific theories was relegated to the background, as merely accessory elements. Had a logical equivalence between diagrammatic systems and formulaic systems been demonstrated in this period (e.g. [2]), we may question whether diagrammatic resources would have constituted acceptable tools for the rational reconstruction of scientific theories by the advocates of the syntactic conception.

From the late 1950s onwards, the syntactic conception of logical positivism gave way to the first proposals (e.g. [9]) to characterize or 'rationally reconstruct' scientific theories not as sets of symbolic formulas but as sets of mathematical structures (set-theoretical, model-theoretical, etc.). In this direction certain physical theories such as Newtonian mechanics would be reconstructed by sets of set-theoretical objects {P, T, s, m, f} where P corresponds to the set of particles, T (real-valued) sets of time intervals, s(p, t) the position of each particle, m(p) the (real-valued) mass of the particle and f(p, q, t) the force that a particle q exerts on p at time t (ibid.). These strategies of characterizing scientific theories as mathematical structures are referred to in the literature as the 'semantic-structural conception', identifying formal theories and models. However, the transition between the syntactic and the semantic-structural conception did not really constitute an advance in the consideration of new representational formats (since both are based on identifying theories as symbolic formulas, either logical or mathematical, respectively), but an advance in the consideration of more expressive formal structures.

It was from the 1980s onwards that philosophers of science such as [5] began to pay attention to the fundamental role of non-formulaic elements (e.g. conceptual schemes, detector images, phase diagrams, etc.) in obtaining scientific knowledge through the use of certain models. This gave impetus to the so-called 'pragmatic conception' of scientific theories and models [3], where models were conceived as epistemically active and intermediary elements between theories and modeled phenomena. On the other hand, in the 1990s there was also a growing philosophical interest in the problem of scientific representation (i.e., what are they, how do they work, etc.) led by [5] and by [7] deflationary proposal, where a representation is characterized by its capacity to (i) 'denote' a phenomenon, (ii) 'demonstrate' certain properties and (iii) 'interpret' its content. In this sense, the pragmatic conception of model-theories and the problem of scientific representations allowed to question the idea that theories should be characterized exclusively as sets of symbolic formulas, what we can here call 'formulaic dogma' of scientific theories.

3 Semantic-Representational View on Theories

However, according to the pragmatic conception à la [3], only scientific models can be considered as format-independent sources of scientific knowledge. According to this conception, what from the formulaic dogma are assumed as ‘peripheral representations’ (e.g. diagrams, icons, images, etc.) would belong to the broad domain of modeling tools but not properly to scientific theories, as formulations of natural laws. In this sense the pragmatic conception presupposes a hierarchy of scientific elements according to their epistemic potential: formulaic theories-laws (epistemically inactive) proto-formulaic theoretical models (epistemically quasi-active) format-independent phenomenological models (epistemically active). The main problem with this hierarchy lies in assuming that diagrammatic representations cannot constitute vehicles of the theoretical principles of the disciplines, but merely tools for the application of these principles. In my proposal I argue against this idea that diagrammatic representations constitute adequate semantic vehicles for encoding theoretical principles. To defend this thesis, I will adopt a semantic conception that directly rejects the ‘formulaic dogma’ about scientific theories. Against the semantic-structural conceptions of [8,9] recently defended a proposal to characterize scientific theories as sets not of logico-mathematical structures (i.e. syntactic and semantic-structural conceptions) but properly of representational models or representations. By ‘representation’ I mean any structure that can consistently encode information about a target phenomenon. Based as a premise on what these authors call the ‘Hughes-Giere-Suarez thesis’ (i.e. all scientific models are representations, regardless of their representational format), [8] argued that scientific theories are composed precisely of sets of representations, or properly a particular subset of all possible representations associated with that theory:

(P1) Theories are composed of a subset M of all models.
(Semantic conception of theories)

(P2) All models are format-independent representations.
(Hughes-Giere-Suarez thesis)

(SR) Theories are composed of a subset of all representations.
(Semantic representational conception)

As can be extracted from the argument above, this semantic-representational (SR) conception of scientific theories presents important theoretical advantages for defending our main thesis (i.e. certain diagrammatic representations are part of physical theories) as opposed to the syntactic and semantic-structural conception. On the one hand, this conception of scientific theories undermines (i) the “criterion of rational reconstruction” of the structuralists, according to which theories can only be identified and, therefore, analyzed by means of logical (syntactic conception) or mathematical (semantic-structural conception) formulas; and (ii) the formulaic-symbolic dogma, according to which the only “rationally legitimate” vehicles of theoretical content are certain types of privileged symbolic formulas. Note that the main difference (as far as our aim here is concerned) between SR and the semantic-structuralist conception (SS, below), is that whereas the latter identifies scientific theories with a subset of models associated with a particular format (formulaic dogma), for SR this subset is completely independent of the representational format of the model:

(P3) Only a subset of formulaic models can be identified with theories.
(Formulaic dogma)

(SS) Theories are composed of a subset of formulaic models.
(Semantic structural conception)

The main advantage of SR for assessing the enormous representational richness of science lies in its ability to get rid of format-centric biases (e.g., historically predominant among syntactic and semantic-structural conceptions) when analyzing the epistemic potential of any model to convey theoretical principles. This does not mean that any representation is valid to be constitutively part of a scientific theory. At this point in our analysis, we argue precisely that the criterion for including a representation in the subset of representations identifiable with a theory is that it contributes to a (i) semantically consistent and (ii) syntactically correct encoding of the theoretical content. Illustratively, for SR particle physics would not be identified exclusively with sets of models or formulaic structures such as {P, T, s, m, f} (i.e. as with SS, above) but with any representation regardless of its format that contributes significantly to the attainment of knowledge by conveying such theoretical content, as in the case of the semantically consistent encoding of 'electric charge' by the direction of the white lines (i.e. up charge-negative, down charge-positive) in a bubble chamber picture (Fig. 1).

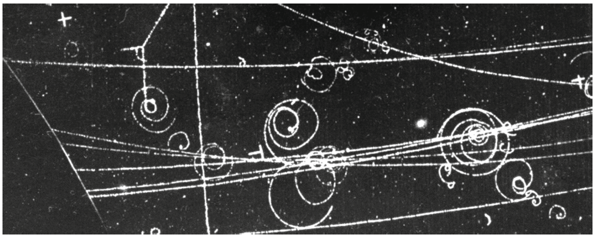

Fig. 1. Bubble chamber picture as a part of particle physics.

4 Case Study: Phase Space Diagrams in Statistical Mechanics

We will now explore phase diagrams in statistical mechanics as a case study (extended in [1]) to demonstrate the potential of the semantic-representational conception of theories in the evaluation of the epistemic potential of diagrams in science. Statistical mechanics is the discipline that studies certain macroscopic behaviors (i.e. an expanding gas inside a container V, see Fig. 2) from the dynamics of its microscopic components of material systems. To achieve this goal, the position and velocity of all the molecules that make up a gas are encoded in what is technically known as the phase space Γ of this system, whose exact values for each moment (or 'microstate') are represented by points x in this abstract 6n-dimensional Γ-space (wherein n is the number of particles, usually $n = 10^{24}$ per mole of substance). This abstract space is usually represented by 'portraits' or 'phase diagrams', which are nothing more than two-dimensional simplifications that remove large amounts of redundant and irrelevant information from the phase space of a system. Within this phase-diagrammatic apparatus, the set of microstates compatible with an observable property of the system (i.e. the volume 1/2V of a gas before it expands) is represented as bidimensional areas or 'macrostates' Γ_m in this phase space. As the gas progressively expands through the total physical volume V of the vessel, the microstates contained in the initial macrostate Γ_m (i.e. phase volume of the macrostate) progressively move through the phase space Γ.

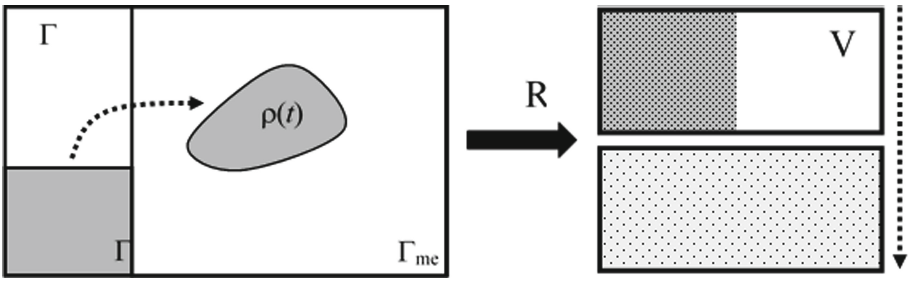

Fig. 2. Phase diagram (left) representing a gas approaching equilibrium (right).

From our semantic-representational conception of theories we can robustly defend that it is possible to employ diagrammatic resources as representational vehicles of certain theoretical principles of statistical mechanics. In particular, the statistical mechanical meaning of the celebrated 'Liouville theorem' would be visually encoded by preserving the two-dimensional dark gray area from Γ_m to ρ(t), wherein the theoretical content of that theorem would be semantically-consistently preserved from a 10^{24}-dimensional phase space to the two-dimensional graphical representation viewable in Fig. 2. In fact, from the framework of the representational semantic conception, certain semantically consistent and syntactically correct devices such as these kind of phase diagrams would no longer be considered as marginal representational practices (as it would make sense to claim from the formulaic dogma), but would be included in the body of the theory itself as a constitutive part of it. Thus, statistical mechanics as a theory would not be constituted by a set of statements set out in a technical textbook, but by a set of valid representational practices with which to obtain meaningful information about a physical field.

To check whether the type of phase diagrams represented in Fig. 2 allow us to convey theoretical content in a semantically consistent and syntactically correct way, let us explore the scenario in which we represent the evolution of an expanding gas in a vessel and also perform a macroscopic measurement during this process. In this case, the phase space of the expanding gas under consideration is divided into three different macroscopic macrostates (Γ_m, $\Gamma_{m'}$ and Γ_{meq}), each associated with a particular value of a macroscopic observational variable such as the volume V, where the macrostate having a larger volume (Γ_{meq}), represented graphically as a two-dimensional area of the macrostates, corresponds appropriately to the thermal equilibrium state of the system. Being a "dynamic" phase diagram, the phase structures it contains represent synchronously three different moments in the evolution of the target system. At the initial time (t_0) the macrostate Γ_m, the farthest from thermal equilibrium, is considered to have a positive and uniform probability measure (light gray) that statistically describes the system at time t_0; this means that the current microstate of the system is found with equal probability at any of the points it contains.

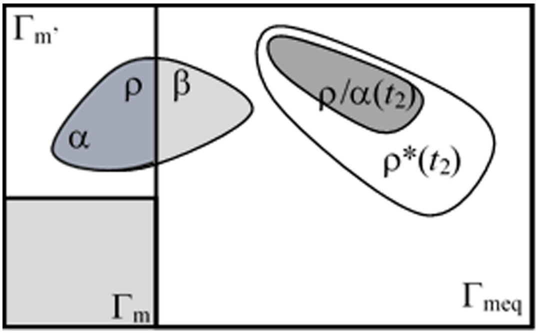

Fig. 3. Phase space representation of the dynamic evolution of a physical system (encoded via a density ρ) in the theoretical context of classical statistical mechanics.

At the beginning of the dynamic evolution of the system, all the microstates contained in Γ_m move along the phase space generating (let say at time t_1) what Shenker and Hemmo call a 'dynamic blob' ρ having a uniform distribution of probability defined over different regions in Γ. At this precise moment, a measurement would be carried out on the macrovariable associated with the macrostates, dividing the dynamic blob into two parts α and β depending on the particular macrostate ($\Gamma_{m'}$ or Γ_{meq}, respectively) in which they are found. Note that the partition of ρ determines the probabilistic results of such measurement. Finally, let us imagine that the macrostatistical measurement results in the value of the macrovariable associated to $\Gamma_{m'}$; then we take into consideration ρ/α (that is, the part of contained in $\Gamma_{m'}$, visually highlighted in dark grey) and let it evolve dynamically until at the moment t_2 we would obtain ρ/α(t2). On the other hand, we take ρ/α and carry out a phase averaging of its probability values along macrostate $\Gamma_{m'}$ (namely, coarse-graining procedure as detailed in Sect. 2) generating a new probability distribution ρ* that will dynamically evolve into ρ*(t_2).

Firstly, we can point out how various graphic resources of the diagram serve to encode in a formal-syntactically correct and semantically consistent way statistical mechanical content. For example, the fact that the area contained in macrostate Γ_m is uniformly light-grey colored can be considered as a graphic-chromatic resource used to encode that the probability distribution defined on that very macrostate will be uniform. Since any agent competent with (i) the syntactic-semantic functioning of this type of phase diagrams and (ii) with the basics concepts of statistical mechanics will be perfect able to access such graphically encoded theoretical content to draw inferences about the target system (e.g. concluding that any two possible microscopic configurations contained in this macrostate will be equally likely to be the actual one), such a diagrammatic element (the uniform grey colouring of Γ_m) may be considered as a valid representational vehicle.

In the same way, other graphic resources such as the area invariance between ρ/α at time t_1 and ρ/α at time t_2 would correctly and consistently encode the meaning of the Liouville principle as a mechanical statistical content (notice that if such an area were to change from t_1 to t_2, then the content of the Liouville theorem would be encoded in an incorrect and inconsistent way). From our semantic-representational conception of statistical mechanics, a well-formed phase diagrams like the one in Fig. 3 would properly render not as an indispensable but as an effective tool for drawing statistical mechanical inferences about the thermal behaviour of certain kinetic systems.

Finally, we argue that from our semantic-representational perspective we can delimit the way in which diverse representational resources (i.e. phase diagrams, in our case study) contribute to produce knowledge (i.e. statistical mechanics). In this sense it can be shown how phase diagrams not only have a merely ancillary role (connected to their greater or lesser usefulness) in obtaining information about the objective thermal phenomenon, but also a constitutively epistemic function. Illustratively, phase diagrammatic representations enhance the comprehensibility of the mechanical statistical content on which inferences are drawn because of its visualizability (or cognitive accessibility). Liouville's theorem is prima facie more comprehensible by means of its visualizable diagrammatic representation (i.e. invariance of the area of ρ/α in Fig. 3) than by means of the symbolic-analytical formula $|\rho/\alpha\,(t_1)| = |\,\rho/\alpha\,(t_1 + \Delta t)|$, since any agent will require more technical and conceptual skills (as well as cognitive processing resources) to access the same statistical mechanical content from the formulaic than from the diagrammatic representation.

5 Conclusion

We conclude by defending that from a conception of scientific theories such as the semantic-representational one of [8] we can evaluate the epistemic potential of certain diagrammatic representations (semantically consistent and syntactically well-defined) as theoretical vehicles. An example of this can be found precisely in the case study analyzed in the previous section, where the semantic-syntactic manipulation of diagrammatic resources allows us to obtain theoretical knowledge in certain statistical mechanical scenarios at the same level as from equivalent formulaic representations. For example, we can satisfactorily explain what a macroscopic measurement consists of through the valid representational resources contained in Fig. 3, explicating that when performing a measurement at t_1 of an observable property (e.g. volume V) of the target system, the whole pre-measurement density ρ collapses in either ρ/α or ρ/β with a degree of probability proportional to the graphically encoded area of each of these post-measurement distributions. We have shown how the capacity to exploit inferential a phase diagram has a direct impact on the possibility of generating mechanical statistical explanations, for example, by making explicit how graphically separating the area of ρ into two non-overlapping regions associated with macrostates $\Gamma_{m'}$ and Γ_{meq} (respectively) at time t_1 could constitute a robust explanation of a macroscopic measurement process in statistical mechanics. In short, our results should be taken as a modest vindication of the enormous representational richness that underlies science, disregarded for decades by the philosophy of science.

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