SYMMETRY INFERENCE IN THE PHYSICAL SCIENCES

by

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A Thesis
Submitted to the
Graduate Faculty
of
George Mason University
in Partial Fulfillment of
The Requirements for the Degree
of
Master of Arts
Philosophy

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Date: __________________________________ Summer Semester 2019
George Mason University
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Symmetry Inference in the Physical Sciences

A Thesis submitted in partial fulfillment of the requirements for the degree of Master of Arts at George Mason University

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ACKNOWLEDGEMENTS

I would like to thank Professor DiTeresi, who shepherded me through so many exciting developments in the Philosophy of Science, and the other members of my committee, Professor Jones and Professor Cherubin, for their patience and for guidance on expressing these ideas and relating them to the other philosophical currents.

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ABSTRACT

SYMMETRY INFERENCE IN THE PHYSICAL SCIENCES

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Symmetry inferences in the physical sciences have material warrants; these warrants can be accounted for in terms of scientific practice and conceptual adaptation. This study is a historical epistemology that provides such an account. It covers the emergence and development of symmetry warrants in the crystallographic research programs of the nineteenth century; it also provides evidence and reasoning undermining alternative accounts that characterize symmetry in mathematical rather than material terms. The study suggests that symmetry concepts adapted in order to reduce the number of arbitrary assumptions and parameters otherwise required by crystallographic research programs to account for an expanding range of physical properties that were being measured with ever-greater precision. The use of symmetry reasoning in these programs lessened the dependence of scientific practice on theory and, by doing so, restrained speculative theorizing, established common ground for practitioners with diverse ontological assumptions, and facilitated experimental progress even where theoretical understanding was weak. Further historical research on the development of symmetry

reasoning in crystallography and its spread from that field to others will reveal whether there are also material warrants for the continued evolution and transfer of symmetry reasoning. The stakes are high because the use of symmetry inference is pervasive, *a priori* reasoning about physical symmetries is common but unwarranted, and errors can be costly.

PROLOGUE

"I think there is interest in introducing into the study of physical phenomena the symmetry arguments familiar to crystallographers," declared Pierre Curie (1859-1906) in a classic paper in 1894. Curie was an accomplished physicist and knew whereof he spoke; he then proceeded to introduce those arguments into physics and to formulate a famous principle of symmetry inference now known as the Curie Principle. Curie's standing in relation to symmetry arguments and crystallography is like that of Kant in relation to philosophy a century before: he had assimilated the earlier traditions and he stimulated the later developments. Physical scientists in the affected fields credit Curie with recognizing the role that symmetry arguments play in the physical sciences and for promoting their use.

Was Curie right to think that symmetry arguments are special and warranted, that they arose in crystallography, and that they can be used in physical sciences? My thesis focuses on these topics. I do not consider the use of symmetry arguments in other fields — such as the arts, law or political theory — nor the use of symmetry for purely descriptive or other non-inferential purposes in the physical sciences.

In this prologue I provide a narrative overview of the case I make in this thesis that symmetry inferences in the physical sciences have empirical warrants. As symmetry inferences are material inferences, I argue that their warrants are found in the processes of inquiry, specifically in the mechanisms by which the concept of symmetry used in such inferences co-adapts with the sciences it supports. Details of the arguments, objections, examples, references, and other scholarly points are reserved for the chapters that follow.

The Concept of Symmetry

We draw our ideas about symmetry from a deep and ancient pool. In Chapter 1 I note a number of the features commonly found in notions of symmetry (such as aesthetic, geometric, algebraic, physical, and abstract features) and the sort of questions we often ask about them. There are, however, no *a priori* timeless verities residing in them that a purely conceptual analysis would reveal for us; it is only by determining how symmetry is used in any particular case that we can hope to unpack its meaning. The point of noting the various features of symmetry at the outset is not to use them as axioms or as any other starting point for my analysis, but just to draw attention to the cultural inheritance that gives us a wide choice of symmetry metaphors, to the need to establish that any chosen metaphor is up to a particular task, and to the possibility we might inadvertently mix up the attributes of one of the notions of symmetry with those properly belonging only to another.

The particular tasks for symmetry I focus on are the inferential tasks. Chapter 1 also includes a number of vignettes of symmetry arguments. These are illustrative only. The point of relating them there is not to establish any *a priori* understanding of what a symmetry argument must be — indeed many of them have led to conclusions known to be false. Rather it is to gesture towards the range of symmetry arguments that have been made historically and to warn against two temptations in particular.

The first temptation is aestheticism. This, expressed in science, is the perennial trope that symmetry is fundamentally an aesthetic command — as if it were the property of a whole constituted of parts in such beautiful proportion as to warrant inferences about the universe. For example, even Johannes Kepler, in his early writings, reported finding such an aesthetic symmetry in the beautifully proportioned geometric figures that 'explain' the orbits of the planets. We rightly dismiss Kepler's argument, but we should also pause to identify any ways in which the argument he offers formally differs from more modern ones. (Is the theory of Supersymmetry in particle physics really "too beautiful not to be true"? What extra credibility does an "elegant" theory have?)

The second temptation is rationalism. We rightly celebrate the symmetry arguments that Archimedes used to derive the thoroughly corroborated body of laws in the field of statics (the branch of mechanics treating balances, levers, and pulleys). These seem to make so much about the world derivable from thought experiments alone, i.e., *a priori.* In like vein, many well-known conservation laws can nowadays be derived from first principles (expressed as a few obvious symmetries). It may be useful to submit (temporarily) to this temptation at the outset by imagining the way the universe must be if it were created according to principles of reason. For it is only then that we can fully empathize with those who have been offended by the behavior of created Nature. (A well-known experiment in electromagnetism in 1830 that did not conform to reasons based on symmetry was described "an intellectual shock"; a well-known experiment in radioactive decay that also defied reasons of symmetry is still described in terms of "violation.") The temptation of rationalism is to imagine that we can be certain about symmetry inferences made *a priori*; we pay a price for this temptation whenever we eschew experiments that could have disabused us of costly mistakes.

The Inferential Warrants of Symmetry

I begin my inquiry proper in Chapter 2 by articulating the task of finding warrants for symmetry inferences. This task requires clarifying what symmetry inferences are (since my introductory comments on inferences were only provisional and motivational) and what warrants are (that is, what justifies them or makes them as effective as they are).

Symmetry inferences that are already warranted on the basis of form alone are not relevant to the question of warrants that depend somehow on the concept of symmetry used. There are in fact many well-known symmetry inferences that are formally valid, such as the mathematics governing chemical bonding and that governing spectroscopy (which can be greatly simplified using rules of symmetry) and the deduction restricting the symmetries that can exist in a crystal lattice. But as the concept of symmetry used in these cases has no bearing on validity of the inference in which they are embedded, I do not consider them further.

Inferences that are specifically *symmetry* inferences are those whose validity depends on the concept of symmetry and also on content, the domain of application. We can exhibit the content-dependence of symmetry inferences in more detail by attempting to classify certain well-known inferences in a formal way.

- Deductive inferences — such as those cited in §2.1 concerning chemical bonding, spectroscopy, and the permissibility of symmetries in crystal lattices — are all formally valid. That being the case, the warrant for asserting their conclusions then depends only on the truth of their premises

- Abductive (hypothetical) inferences — such as conjectures about the internal structure of crystals on the basis of observational data on crystal properties — are not *formally* valid. Their conclusions are not warranted by logic but have to be tested empirically. Even then, any corroborated conclusions remain underdetermined by observational data, since many hypotheses would be consistent with it. It would be very useful to have a formal 'logic of discovery' to funnel one's conjectures towards those with the highest prospects of being corroborated empirically. However, no such formal logic has been found, nor is there any reason to believe that one might be.
- Inductive arguments are likewise not *formally* valid. And again, there are no formal rules either for distinguishing strong from weak inductive inferences, nor any reasons to think that any are possible. Chapter 2 highlights a famous inductive argument that concerns symmetry, namely the argument Louis Pasteur (1822-1895) made, on the basis of a very small sample, to associate molecular asymmetry, living processes of production, and optical activity.

If there were a way to distinguish strong symmetry arguments from weak ones, it would depend on what one is talking about, the concepts used and the domain of their application. Any such way lies in the realm of material logic, the inferential practices of historically situated inquiries, and it has to be discovered empirically. A warrant for material inference then would be an explanation for the degree of inferential success realized or expected. For syllogisms, warrants are found using formal techniques and expressed in terms of rules. But for symmetry inferences, because they are material inferences, we need to seek explanations empirically in terms of the inferential practices of inquiry. As inquiry is historically situated, any such explanations would be historical too.

I distinguish below three kinds of material warrant, i.e., three kinds of explanation, each corresponding to the success of a different kind of inference. (Although I express and illustrate each of them in relation to symmetry, warrants of these kinds could be developed for other kinds of material inference as well.)

Projectable Warrants

The first, which I refer to as the projectable warrant, is the explanation for the continued success of repeated applications of what is recognizably the same inferential practice within a research program at a given stage of its development. This warrant cannot, of course, depend on a formal analysis of the propositions used but must depend on context of the inquiry in which those propositions find their meaning. In §2.4, I illustrate how this works using the example cited earlier of Pasteur's famous induction of 1860 that associated lack of symmetry in molecular and crystal form with living production processes and resultant ability of solutions to rotate the plane of polarization of light. Pasteur's inference was clearly a material inference. (As a material inference it was also fallible; this is illustrated by the fact that Pasteur's first attempt was to argue on the basis of the concept of form, a basis he had to discard in favor of the concept of symmetry when inferential success eluded him.) The same inference pattern continues to apply to substances other than the particular ones on the basis of which the original inference was made. In that sense, it is “projectable.” Inspired by Pasteur’s experience, Ian Hacking’s concept of self-vindication in experimental practices, and Bas van Fraassen’s selectionist explanation for the success of science, I set out to account for the projectable warrant of symmetry inferences in terms of conceptual co-adaptation. I seek evidence in the historical records for the mechanisms by which the symmetry concept has been adjusted over time and in tandem with the science it supports.

Evolvable Warrants

The second, which I refer to as the evolvable warrant, is the explanation for our continued success in developing new projectable warrants on the basis of concepts that are recognizably variants of earlier concepts of symmetry. These variant concepts differ from the earlier ones, of course, but there is a continuity as well that we recognize by calling all of them symmetries. Unlike the projectable warrant, which applies at a particular stage in the development of a research program, the evolvable warrant stretches over time as new problem situations arise.

I draw an analogy between the evolvable warrant of symmetry (i.e., its ‘surprising’ utility) and two other evolvable warrants that have already been addressed in the literature: that for the ‘miraculous’ success of science and that for the ‘unreasonable’ effectiveness of mathematics. The most promising explanations given for the latter two were based on selection. Below, I speculate on a similar mechanism for the evolvable symmetry warrant too.

Transferable Warrants

The third warrant, which I refer to as the transferable warrant, is the explanation for successful transfers of symmetry reasoning from one domain to another. Perhaps these warrants are rooted in shared laboratory cultures or perhaps in analogous relationships among system elements in both the source and target domains. Transfer is clearly what Pierre Curie had in mind in his 1894 paper — transferring inferential forms from crystallography to other physical sciences, specifically electricity and magnetism outside crystal boundaries. In the twentieth century it has been abundantly evident that the transfer of symmetry reasoning among the physical sciences has often been very successful. Although transfer warrants are beyond the study period of this thesis, which ends with Curie's paper, they are important enough to merit investigation in their own right.

The Historical Development of Symmetry

In Chapter 3 I focus my attention on where the evidence for the mechanisms underpinning symmetry warrants may lie. Inquiry comprises practices and these have a history; I therefore need to examine the inferential practices that involve symmetry over time. Building on the claim, which has been accepted since Curie's time, that the scientific concept of symmetry emerged in nineteenth-century crystallography, I focus my case study on this field and on this time period. That scope is enough to evaluate the empirical thesis of conceptual co-adaptation and to evaluate plausible rival claims of *non* co-adaptation that are based on developments in associated branches of contemporary mathematics.

There are no historical epistemologies of symmetry that I can use directly for my case study on the inferential uses of symmetry, even though there are several excellent histories of symmetry written for other purposes. I aim to model my effort therefore on the best-practice historical epistemologies about concepts related to symmetry, such as objectivity and probability, and to treat the similar kinds of issues.

Inferential Practices

Best-practice histories of epistemic concepts show how practices give meaning to concepts. To use that observation in the case of symmetry, I focus on the practices of the main protagonists in nineteenth-century crystallography, René-Just Haüy (1743-1822) and Christian Samuel Weiss (1780-1856), and to some extent on those of their predecessors, associates, and successors. Groups of related practices constitute research programs; to facilitate the analysis of research programs, I borrow a number of distinctions and conceptual resources from Imre Lakatos (1922-1974) who, unlike Karl Popper and Thomas Kuhn, the most renowned of his rivals, takes a historical approach without sacrificing conceptual continuity in successive programs and he adopts the research program as the unit of analysis rather than the individual theory or claim.

Conceptual Continuity

Best-practice histories also show that there are conditions that allow one to say of a concept that it has a history. That is, they distinguish between an identifiable concept changing over time and a series of unrelated concepts succeeding one another. That will be important for symmetry, as it does seem that variants of the symmetry concept have been used sequentially; I will therefore need to show where successive concepts are similar — and to be aware of where they are different in order to minimize the danger of inadvertently and inappropriately ‘dragging’ the properties of an earlier conception of symmetry to a later one.

Mechanisms of Change

Lastly, the best-practice histories generally posit mechanisms to explain the stability of, or changes in, a concept or inferential practice over time. It is crucial for establishing a projectable symmetry warrant, conceived as an account of material inferential success, that we can do this. This means, first, establishing that the inferential practices are in fact successful and, second, identifying mechanisms for the adjustments that entrench successful practices or lead us away from unsuccessful ones.

Inferential *practices* are successful if they lead to successful inferences whose success is both general and principled. First, while any single inference is successful if observed data match its conclusion, an inferential practice would need to be generally successful. (Lakatos is again helpful in this regard because of his acceptance of the research program as the unit of analysis, rather than an individual model or single experiment.) Second, for inferential success to be a useful criterion, the matching of observations to conclusions has to be done in a principled (i.e., non-arbitrary) way. This is an important caveat, one we owe to yet another distinction that Lakatos draws. This is the distinction between the 'hard core' of the research program (the key commitments and practices that define the program and which are therefore strongly defended) and the 'protective belt' (various ancillary assumptions, some of which could be sacrificed if necessary to defend the hard core). Lakatos rightly recognizes that vastly more observations can be 'matched' to model outputs if we were licensed to make arbitrary adjustments to the protective belt. Typical appeals to the protective belt include assumptions about the range of experimental errors likely to be encountered, claims about observations that are actually artifacts of the instruments used, and the uniformity or irrelevance of other experimental conditions. But for inferential success to be at all useful, such appeals have to be principled, i.e., restricted to those based on sound scientific grounds according to principles that are themselves general (rather than *ad hoc*). When this can be done, we have what Lakatos terms a progressive research program. Where it cannot, we have a degenerating one. In his framework, inferential failure is not a simple mismatch between an inference and observational data but the *inability to make such matches other than by appeal to arbitrary or scientifically unwarranted assumptions or to* ad hoc *adjustments to the protective belt.* Such degeneration often presages a problemshift, the construction of a new research program, with its own 'hard core.' There is historiographical evidence for the progressiveness or degeneration of the research programs in the study period.

The mechanisms of conceptual adjustment we are looking for are those that entrench successful inferential practices or lead us away from unsuccessful ones. I shall not dwell on 'external' mechanisms that may have temporarily shaped research programs, such as career opportunities, funding sources, and personal traits; in the case of crystallography, for instance, Franco-German nationalist rivalry in the Napoleonic era and Haüy's well-known resistance to criticism certainly played such as role. Rather, I will focus on the more enduring factors affecting the scientific problem situation itself, such as the increasing precision of instruments and newly discovered physical phenomena.

Taking a research program approach keeps open the hypothesis that it was the *entire research program*, including the scientific model in which the symmetry concept was embedded, that is responsible for inferential success or failure — not just the symmetry concept in isolation. That is, inferential success is due to symmetry's *co*-adaptation, not just its adaptation. Needless to say, if the historical record were to show that the full burden of conceptual adjustment fell on the scientific model, that no burden fell on the concept of symmetry, or that any adjustments in the concept of symmetry were fully accounted for in some other way, such as by mathematical research programs alone, this hypothesis would be disconfirmed.

Historiographical Issues

In addition to these best-practice considerations for a historical epistemology, one needs to be aware of potential historiographical pitfalls.

One pitfall is anachronism. While there is always a general risk of inadvertent anachronism, there are some specific issues in the case of crystallography that are worth noting. In §3.5, I raise ones about the nature of that science, the use of terms like 'atom' and 'molecule,' and the historical ambiguity in the term 'form.'

Another pitfall is rational reconstruction. This is the risk that a historical epistemology will slip into being a history that not only highlights the inner logic of the discipline but that in doing so it actually misrepresents the chronology or historical processes. In §3.5, I set out the situations where rational reconstruction is not only legitimate but also useful; history, though, is not one of them. I have two reasons for raising this issue explicitly. The first is that I have made free use of many of the conceptual tools of Lakatos; since he is sometimes interpreted as espousing the rational reconstruction of history, it is important to say that this is not my aim here. The second is that, because I borrow certain categories and distinctions from Lakatos, I may be inadvertently imputing the use of such categories and distinctions to the historical actors I describe. The most important of these worries is about the process of conceptual adjustment. There is historiographical evidence though that contemporary reviewers of crystallography research also evaluated rival research programs in this way, i.e., that they preferred research programs with fewer *ad hoc* assumptions to ones with more.

The Empirical Construction of Symmetry

The case study in Chapter 4 shows, as Curie implied, that the concept of symmetry emerged and developed in nineteenth-century *crystallographic* research programs and that because this concept co-adapted with empirical science to maximize inferential success, the inferences made on the basis of that concept, although fallible, are empirically warranted. The study also discredits claims that the scientific concept of symmetry was a mathematical one that had been transplanted from *mathematical* research programs.

The historical case material is presented as a historical epistemology that tries to emulate the best practices listed above, namely those that reveal inferential practices, conceptual continuity, and the mechanisms of change. I analyze a sequence of research programs in crystallography according to a broadly Lakatosian framework by: situating each historically; identifying the problem situation and the symmetry concepts used; articulating the positive and negative heuristics defining the program, especially those concerning the treatment of anomalies; and noting any progressive or degenerating features that could have prompted the adaptations maximizing inferential success.

Crystallography

I begin the case study with a brief survey of the state of crystallography just prior to the nineteenth century. This is because those pre-scientific programs bequeathed the scientific ones that followed both with a problematic that served throughout the nineteenth century and with conceptual resources on which they could draw. The important problems for crystallography had long been:

> Why do crystals have the number and variety of shapes they do?
>
> How can crystal shapes be classified?
>
> What is the relationship between crystal properties and their inner structure?

The most important conceptual resources offered were the concept of symmetry (albeit an aesthetic one concerning fitting proportions that had normative force) and the concept of substantial form (the form that makes something the thing it is, as opposed to its merely 'accidental' features).

Projectable Warrants

Instead of summarizing in this prologue all aspects of the research programs covered, I will focus selectively on the mechanism driving change in the concept of symmetry. All the crystallographic programs addressed the degeneration in rival programs as well as any perceived in their own. Evidence of degeneration is found in the arbitrariness of program specification and in the maneuvers made to protect the 'hard core' from anomalous observations. Where such maneuvers cannot be made in a principled way — if, say, one has to resort to using many brute facts, free parameters, *ad hoc* assumptions, or arbitrary postulates to do so — the research program is clearly degenerating and this presages its ultimate replacement. Concepts of symmetry may be a useful defensive maneuver because they offer ways to deem otherwise disparate features equivalent, thereby at least reducing the number of free parameters needed to specify a system.

Jean-Baptiste Louis Romé de l'Isle (1736-1790) had already attempted to reduce crystallographic arbitrariness towards the end of the eighteenth century. He proposed a way to reduce the vast number of observed crystal shapes (each of which was otherwise just a given) through making a principled distinction between accidental and substantial forms. He had observed that crystals had natural cleavage planes and that their shapes can be altered in lawlike ways by beveling edges and truncating corners. Such alterations in the shape were of course 'accidental' in that they did not change either the composition or any other properties of the crystal. Despite this insight, his program was roundly criticized for its own arbitrariness: the initial choice of a primitive form.

Haüy, by contrast, offered a model of internal structure that *explained* the observed crystal shapes and *explained* why the vast majority of conceivable shapes do not occur in nature. His model was a 'molecular' account; crystals were regarded as assemblies of identical building blocks (primitive forms) stacked up in lawlike ways. That meant that researchers would no longer have to accept each crystal shape they observed as just another brute fact. Furthermore, Haüy's primitive forms purportedly escaped from the arbitrariness of his predecessor's primitive forms. That was for two reasons. One was that Haüy had an empirical method that he claimed could determine primitive form — repeated cleavage, a process that typically resulted in an asymptotic form, one that no longer changed. The other reason was that, as he later posited, an aesthetic symmetry supposedly limited and explained the range of primitive forms that could be found this way. This model made the testable prediction that the permissible crystal shapes were those that could be generated by stacking blocks of a particular size and a particular primitive form; given an empirically determined primitive form and a postulated way of stacking them (a 'Law of Decrement') he could predict which shapes would, and which would not, be possible in nature. Haüy's program was theoretically progressive because it reduced the number of arbitrary parameters and it was empirically progressive to the extent that its predictions about shape were (initially) empirically corroborated. Haüy's program though became a degenerating one when precise measurements required abandonment of his aesthetic symmetry and once it was clear that newly studied crystal phenomena, particularly those with directional attributes, could no longer be absorbed in his model in a systematic way.

Subsequent research programs in crystallography proceeded through much the same cycle — a progressive change in the way of viewing the problem situation that eliminated or reduced the arbitrariness of the preceding program; a new heuristic that included the use of a revised concept of symmetry; anomalies and appeals to the 'protective belt.' I trace the successive research programs of Weiss and other members of the German school, and of some later researchers in the French tradition before the time of Curie. At each step, not only was the concept of symmetry refined, but also the tacit understanding of its application was strengthened. The reliability of symmetry inferences thus improved through continual adaptation.

Rival Claims that Symmetry Warrants are Mathematical

I then pause to consider rival claims that symmetry warrants are not empirical, as I have argued above, but mathematical. The grounds for these claims are that the concept of symmetry originated in mathematics and that it belongs in that field of inquiry. I articulate what I take to be the most plausible variants of this claim. All but one of these claims is, to my knowledge, implicit. But because they are widely held and quite plausible they need to be examined explicitly.

The first claim (one that has been advanced in the literature) is that the scientific concept of symmetry arose in solid geometry, where the French mathematician Adrien-Marie Legendre (1752-1833) defined it in 1794. However, apart from the timing of Legendre's definition (just before Haüy's scientific program in crystallography) and its resemblance to modern definitions, there is no historiographical evidence of its application to or influence on the empirical progress of crystallography in the early period (1801-1830) in which various concepts of symmetry were adopted. In any case, Legendre's definition of the concept of symmetry differs from the ones used by the earliest crystallographers: his definition concerns the conditions under which two three-dimensional shapes that are not superimposable are nevertheless deemed equivalent, and that concept was not used until much later (by Pasteur).

The second claim (one that is probably more widely held) is that the scientific concept of symmetry arose in group theory, where another French mathematician had developed principles of symmetry inference, Évariste Galois (1811-1832). This claim also has initial plausibility, especially if we recall just how pervasive group theory has become in the physical sciences. But group theory was not available before 1830 (that is, after concepts of symmetry had developed in crystallography) and not widely used in crystallography until much later in the century. (We must be careful not to accept the rationally reconstructed group-theoretic accounts of early crystallography as being historically literal.)

The last mathematical claim I examine concerns vector analysis, whose role in shaping the symmetry concept is a little less direct. On the one hand, vector analysis is closely related to an important symmetry operation used in theories of the physical sciences (namely, the operation of rotation). This is because vector analysis generalizes the formalism used for describing and manipulating rotations in two dimensions into a formalism that can be used in three dimensions. On the other hand, the origins of vector analysis are indisputably mathematical — it arose in a research program in number theory. But, ironically, what may seem like a triumphant mathematical warrant, is actually a further testament to the role of empirical science in shaping the concepts the sciences use. This is because the original (mathematically derived) vector analysis was not merely cumbersome; its interpretation in terms of three-dimensional space was disastrously inept. So much so that the vector analysis used in the sciences today is a bespoke one, completely rebuilt with a scientific purpose in mind by physicists in the late nineteenth century.

In short, the concept of symmetry used in the physical sciences developed in response to the inferential needs of the sciences, initially those of crystallography. It did not develop in response to any purely mathematical imperatives,

Conclusion

The case study shows that material warrants for symmetry inference can be expressed in terms of inferential practices and conceptual adaptation. I was able to track the role of symmetry in the development of crystallography and also to characterize changes in the symmetry concept as responses to selective pressures on research programs to mitigate arbitrariness.

As discussed in Chapter 5, additional lessons can be drawn from adventitious findings and from reflections on the development of symmetry over time. An important, but unanticipated, lesson is that as symmetry concepts rose in importance, ontological commitments declined. Aesthetic and geometric concepts of symmetry initially had instrumental roles: for Haüy they were in the protective belt to defend a particular molecular theory of matter. But later the algebraic concept used in Weiss's rival research program was eventually what came to define it, not the metaphysics that had originally inspired it. One salutary effect of this 'ontological restraint' was that experimentalists had more freedom to collaborate and make progress without having to defend a metaphysical position. This, for example, led to a fruitful union between crystal lattice theory, the ghost of French molecularism, and mathematization, the ghost of German polar theory. Another salutary effect was that considerable progress could be made even in the absence of a theoretical understanding of matter, electricity, and light. To that 'principled ignorance' we owe the discoveries of optical isomerism by Pasteur in 1848 and piezoelectricity by the Curie brothers in 1880.

The historical procedures described in this case study were used to establish the projectable warrants but, as I speculate in the concluding chapter, could equally well be applied to establishing the others (§5.4). It behooves us to understand the nature of symmetry inference as well as we can, not only because the philosophical payoffs could be significant, but because the symmetry-based investments and research efforts in the sciences are large.

1. THE CONCEPT OF SYMMETRY

In this thesis I examine the warrants for symmetry inferences in the physical sciences. For orientation and motivation, I consider in this first chapter some commonly encountered features of the concept of symmetry used in such inferences and offer samples of historically influential symmetry inferences in the physical sciences.

1.1 Some Common Uses of Symmetry

To indicate the scope of this study, I note some of the ways the concept of symmetry is encountered. These illustrations are informal and provisional, merely to provide initial orientation. Nevertheless they should alert us to the occurrence of common features in the way symmetry is used, which would make it useful to consider how they might be related historically. They should also alert us to the concomitant danger that features properly ascribed to one way of using symmetry might, on occasions, be inadvertently and incorrectly ascribed to another.

Typically, when we pose questions of symmetry, we assume some kind of common basis for the measurement of multiple elements and have some kind of judgment in mind. But there are many different ways in which this is achieved. Imagine the elements are the separate features of a building, various triangles in a plane, or alternate visual perspectives of a crystal. We may be relating those elements alternately in terms of their proportionality, their ability to be superimposed, or the prospects of transforming one into another by some mathematical operation or change of perspective. Depending on whether that relationship is seen in a particular case to be 'ideal,' 'exact,' 'indistinguishable,' or whatever, we may then judge the object or set of objects to be 'elegant,' 'congruent,' 'equivalent,' and so on. The end result is normative: the object is praiseworthy or the inference merits acceptance, say.

To understand the search for warranted assertability more concretely, note the different ways in which we commonly regard symmetry:

- Symmetry has long been regarded aesthetically. Consider, for example, the parts of a building (architectural features such as doors, windows, ceilings, and so on). The scale and positioning of these elements can be measured and the stipulated relationship we are interested in is proportionality. The measured ratios of various elements to other elements can be compared to those constituting 'ideal' balance. If the ratios are close to ideal, the elements may be judged 'appropriate' and the building as a whole 'elegant.'
- Symmetry is often interpreted geometrically. Consider, for example, triangles in the plane. Let us move them around and try to superimpose one on another. When the fit is exact, the triangles are 'congruent' and we infer that geometric properties of one apply equally to the others. This is an example of an early technique known to the ancient Greeks as "an ἐφαρμόζειν proof — superposition — literally placing one thing on top of the other to show equivalences" (Hahn 26-27). We now take such symmetry inferences for granted.

- Symmetry is sometimes meant algebraically, as a transformation of one's visual point of view. Consider the different perspectives one can have of one and the same near-perfect snowflake. The stipulated relation in this case is a 'transformation of the coordinate system,' that is, a particular change of viewpoint, such as a rotation through successive angles of 60° about an axis perpendicular to and through the center of the snowflake. In this particular example, we would judge the snowflake's appearance (or some other measurable property) after each such rotation to be the same; we would say that the snowflake has 'sixfold rotational symmetry'; and we would refer to the transformation of viewpoint itself as an 'invariance.' An object without any algebraic symmetry in this sense will look the same only if we do not change our perspective at all. An object without algebraic symmetry could still be said to be symmetric in a geometric sense though, provided it had been assembled from congruent (geometrically identical) parts — cubes, say.
- Symmetry can be exhibited logically. Consider representations of two separate problems within the same scientific model. For the sake of definiteness, assume the problems are to calculate the shortest distance between two specified points. The representations of this problem comprise only those aspects of the problem situation that are deemed to be 'relevant' to the solution, i.e., they disregard certain features (like the color of the object) in some principled way. The remaining features are presented on a common basis, their logical or mathematical form. The stipulated relationship is one of comparison. If the representations meet the criterion of equivalence (that of being 'essentially the same problem') we would claim that the

> problems are 'symmetric' (that is, have 'essentially the same solution' too). The use of symmetry arguments like this are of great practical importance when a hard problem and an easy one are symmetric in this sense.[1]

The idea of symmetry implicit in scientific literature today generally follows the algebraic conception, although most are rather opaque until actual examples are treated. One example, from a theoretical physicist, is: "Symmetry is immunity to a possible change" (Rosen 2010 *Symmetry Rules* Sn. 1.1, p4; Sn. 12.1, p283). A fuller description comes from a chemist:

> An action that leaves an object looking the same after it has been carried out is called a symmetry operation. Typical symmetry operations include rotations, reflections, and inversions. There is a corresponding symmetry element for each symmetry operation, which is the point, line, or plane with respect to which the symmetry operation is performed. (Atkins, Sn. 11A.1, p448)

French mathematician, Adrien-Marie Legendre (1752-1833) offers yet another: "Two equal solid angles which are formed (by the same plane angles) but in the inverse order will be called angles equal by symmetry, or simply symmetrical angles" (Legendre [1794] 1817, p.155 ; qtd. In Hon, *From* Summetria 2), purportedly a definition of symmetry that is id entified by Hon and Goldstein as "revolutionary" (*From* Summetria 2). More recently, German mathematician Hermann Weyl (1885-1955)

[1] This illustration is based on an example described in much more detail by van Fraassen in *Laws and Symmetry* (234-39).

retroactively defines symmetry in terms of its recent mathematical expression in terms of group theory (45); a paraphrase of his definition that leaves out the technical terms is: "For a given configuration of the elements of a system, those transformations that leave the system unchanged form a group and that group exactly defines the symmetry possessed by the system."

We can reserve judgment on the various conceptions of symmetry till later; for now let's just take note of a few claims supposedly based on inferences made with those conceptions.

1.2 Sample Inferences Based on Symmetry

The following is a sample of historically influential arguments that were based on symmetry. These are not 'paradigms' in the sense of examples that should be followed; indeed, many are no longer convincing and some of the claims are known for other reasons to be false. But they have nevertheless motivated the search for general symmetry principles and several even create a sense of wonder. They have been selected in part to represent a wide range of arguments and in part to highlight important differences — some arguments appear *a priori* and 'obvious,' while others lead one to view certain empirical outcomes as 'counter-intuitive.'

Anaximander of Miletus (ca. 610 - ca. 546 BCE) inferred that the Earth is stationary because of a logical equivalence: it is equally distant from the 'extreme points' and so any argument for it to move in one direction is logically symmetric to any argument for it to move in another direction. Aristotle gives us this summary:

> [T]here are some, Anaximander, for instance, among the ancients, who say that the earth keeps its place because of its indifference. Motion upward and downward and sideways were all, they thought, equally inappropriate to that which is set at the centre and indifferently related to every extreme point; and to move in contrary directions at the same time was impossible: so it must needs remain still. (*De Caelo* 295b 10-16; DK 12A26)

Anaximander's conclusion, although disputed by many, persisted for thousands of years (whether or not that was because of his argument). While it is easy to dismiss it now as being silly, given our post-Copernican knowledge, the argument is very interesting methodologically as it is not superficially all that different from more recent arguments in other material contexts, like probability theory and particle physics.

Archimedes of Syracuse (288 - 212 BCE) invoked a similar principle of inference to support his postulate about the balance, namely:

> 1. Equal weights at equal distances are in equilibrium, and equal weights at unequal distances are not in equilibrium but incline towards the weight at the greater distance. (Heath 189)

On the one hand this seems like a trivial example of logical symmetry: whatever argument one can make for a balance with equal weights at equal distances from the fulcrum to tilt down on the right (say) can be made equally strongly for the balance to tilt down on the left. Other reasoning however shows that if the balance arm moves down on the right it would have to lift *up* on the left. But (to recycle Anaximander's words) "to move in contrary directions at the same time is impossible," so one can infer from the symmetry of the way the problem is described[2] that the arm must remain in equilibrium. Yet on the other hand it seems surprising: Archimedes succeeded when Anaximander did not. Archimedes did not use nor did he apparently need any empirical understanding of gravity (other than the fact that it acts downwards). By using various postulates like the one above he could develop a science of mechanics that seems entirely *a priori.*[3] The system was devised in the spirit of Euclid's deductive method, but was nevertheless immensely useful in practice. Can one dream of a foundational physics that is entirely *a priori*?

Hans Christian Ørsted (1777-1851) also took a risk on the way forces operate but, unlike Archimedes, his symmetry-based conjecture was not borne out. His famous experiments were designed to detect the effect of forces generated by an electric current on a magnetic needle. The magnetic needle of a compass aligns itself in a north-south direction with the Earth's magnetic field and gravity of course acts vertically down. Ørsted considered the case of an electric current running from south to north, above and parallel to the compass needle and inferred, from the symmetry of the situation, that the

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[2] In the implicit model of the system, there are a number of potential asymmetries that are not 'relevant to the solution' and which can therefore be ignored, e.g., if it were the case that the color of the arm on the right is red and the arm on the left is blue.

[3] No one would ever request a grant from the National Science Foundation to test Archimedes' balance postulate for 10 lb. cannonballs, 20 lb. cannonballs, and so on. But is this because his answer is obvious *a priori* or because the operations of gravity have been so thoroughly corroborated empirically?

current's effect (if any) on that needle would obviously be in the same vertical plane: any argument he could make for it to move right (say) he could make equally well for it to move left. Hence, one would conclude, the needle can move neither right nor left but only up, down, forward, or backward. Reportedly, Ørsted wasted eight years on other experimental configurations until a chance 'mistake' revealed that the needle actually moves left (Altmann 32). The physicist Ernst Mach (1838-1916), who had reflected deeply on the Archimedean system, warned that we should not be led by its success to "create a new mysticism out of the instinctive in science and to regard this factor as inevitable" (27).

> Even instinctive knowledge of so great logical force as the principle of symmetry employed by Archimedes, may lead us astray. Many of my readers will recall, perhaps, the intellectual shock they experienced when they heard for the first time that a magnetic needle lying in the magnetic meridian is deflected in a definite direction away from the meridian by a wire conducting a current being carried along a parallel direction above it. The instinctive is just as fallible as the distinctly conscious. (27)

It does matter how the world is and this historical episode is a paradigmatic way to show that this cannot be known *a priori.* Altmann not only draws attention to this but further laments that same error was also committed 130 years later when a certain experiment on the radioactive decay was long delayed by "preconceived rather than experimental ideas about symmetry" (36), i.e., because the outcome seemed obvious, the way the outcome of an Archimedes balance experiment seems obvious. (When the experiment in question was finally performed in 1957 it strongly contradicted the result expected on the basis of symmetry considerations.)

Niels Abel (1802-1829) was a mathematician and not required to consult experiment before drawing his symmetry inferences. He was concerned with discovering whether equations containing algebraic expressions raised to the power of five or more can always have solutions. Solutions to quadratic equations (those with expressions raised to the second power) had been available since the time of the Babylonians and those of the cubic (third power) and the quartic (fourth power) since the Renaissance; explicit solutions were available as formulas that used rational numbers as well as 'radicals,' that is, fractional powers of numbers, like square roots, cube roots, and so on. Abel's initial aim was to find solutions to the quintic (fifth power). Abel inferred in 1824, using a *reductio* argument, that in fact no explicit general solution is possible. In what looks like a logical version of the Archimedes' balance argument, he assumed that if there were explicit solutions to the quintic then the symmetry of the permutation of the solutions would lead to a contradiction. Recall that for Archimedes a conclusion that was a physical impossibility meant 'no tilting,' whereas for Abel a mathematical contradiction meant 'no solution.'

Today, Abel's proof is mostly known through the more general and more profound symmetry argument provided just a few years later by the French prodigy, Galois. This was a triumph of abstract algebra and that algebra is now the language of symmetry in the physical sciences, but does the certitude of the mathematics transfer to these sciences?

Some of the arguments above have been empirically corroborated and others have not. What distinguishes and warrants the successful ones?

2. THE INFERENTIAL WARRANTS OF SYMMETRY

In this second chapter I begin my inquiry into what warrants symmetry arguments in the physical sciences (i.e., what makes them so surprisingly effective) by clarifying what a symmetry argument is and by clarifying what would constitute a warrant for asserting its conclusion.

First, given the variety of questions one can ask of symmetry inferences, I try to classify inferences we might encounter (§2.1). I note that formally valid syllogisms cannot cover the scope of what would be needed for scientific inquiry. One initial response to this is to re-arrange the propositions that constitute a syllogism, the way Peirce does, in order to bring abduction (conjecture) and induction into the classificatory scheme as well. But I note that this will not bring symmetry inferences into a *formal* scheme because, as is generally accepted, there are no formal warrants for abductive and inductive inferences nor any reason there ever will be. I illustrate this in the case of symmetry inferences.

Second, I argue that warrants are grounded in material logic. Material logic is not universal; it is dependent on the domain of use or discourse. Inferential practices are warranted empirically and in turn give meaning to the concepts, like those of symmetry, used in the inferences made (§2.2).

Third, I distinguish types of material warrant we have been seeking. Symmetry inferences are material and historically situated and their warrants will be based on reliable inferential practices. What I term the 'projectable' warrant is what justifies the repeated use of a particular symmetry concept in inferences. What I term the 'evolvable' warrant is what justifies the repeated modification of the symmetry concept to accommodate changes in the inferential needs of an evolving science. And what I term the 'transferable' warrant is what justifies the transfer of modes of symmetry inference from one domain to another. In this thesis, the case study material demonstrates the operation of the projectable warrant and provides grounds for speculating about the mechanisms underpinning the other two.

Finally, I provide examples to illustrate what would be expected of such warrants. I consider how the history of adaptation of the symmetry concept underpins the projectable warrant, using the symmetry argument made by Pasteur (§2.4). I then consider how mechanisms of conceptual adaptation could underpin the evolvable warrants in symmetry and in two conceptually parallel cases, one concerning the success of science and the other the effectiveness of mathematics (§2.5). I do not consider the transferable warrants explicitly, as they are beyond the scope of this study, but make some remarks in the concluding chapter.

2.1 The Classification of Symmetry Inferences

Traditionally, an argument comprises premises and an inference that purportedly warrants a conclusion. When the premises are 'true' and the inference is 'valid' we regard the argument overall as 'sound.' Aristotle classified the inferences that were valid in virtue of their form. This classification, however, does not cover the full scope of inferences we typically make in scientific inquiry; for example, generating a scientific hypothesis and testing its predictions against observations involve probabilistic inferences that cannot be formally valid.

Because traditional argument forms do not cover the full scope of inferences used in scientific inquiry, Charles Sanders Peirce (1839-1914) introduced a broader classification of inferences that do (C.P 2.619ff). In his formal schema there are three phases of scientific inquiry (conjecture, prediction, and confirmation) and these phases are associated with distinct types of inference (abduction, deduction, and induction, respectively). Those inference types can be expressed as re-arrangements of the propositions of a traditionally valid deductive syllogism (major premise, minor premise, and conclusion). According to Peirce, we begin inquiry with abductive inference, when we move from particular observations to an explanatory hypothesis. We then use deductive inference to determine a range of observational consequences of that hypothesis, consequences that would correspond not only to the original observations but also to newly predicted ones. Finally, we use inductive inference once experiments have been performed to determine whether the sample observations can confirm the wider population of deductive consequences. Only deduction would be formally valid of course, so we still need a basis for judging the validity of abductive and inductive inferences. Providing such a basis presents well-known problems for scientific inference quite generally, but we can see how it plays out specifically in the case of symmetry inference in the following illustrations.

Deductive Inferences

Deductive inferences, in the Aristotelian sense in which they are formally valid, do not in themselves pose any *philosophical* issues specific to the use of the symmetry concept in the physical sciences. This is because their validity would not be affected by replacing references to symmetry with placeholders: the soundness of symmetry arguments employing a valid deductive inference depends solely on the truth of the premises.

To see this, consider the role of symmetry arguments in chemical bonding as an example of deductive symmetry inference. This argument is rather technical, but the essence is given as follows. In the quantum model, atomic bonds are possible only where the electron orbitals of the bonding atoms positively overlap, i.e., where those overlapping orbitals represent some finite probability of the electrons' being between the atoms. This is expressed *mathematically* in the theory as the condition that the integral over space of the overlap function is non-zero. Quantum mechanical calculations are typically very difficult, but there are mathematical techniques, based on symmetry considerations, that can show in advance that particular overlap integrals will necessarily be zero. In such cases, one can avoid what in general would be very arduous calculations and reliably state that those overlaps do not represent chemical bonds. Thus: from premises about symmetries of the electron orbitals we can make deductive inferences about bonding; but the empirically relevant issue is how we arrived at those premises in the first place, not how we then use them in deductive inferences like those above.

A similar example is the symmetry argument that has been so successfully deployed in spectroscopy. Electromagnetic waves are absorbed and emitted by atoms and molecules when the energy of the photon corresponds to the difference in the energy levels of their initial and final states. It turns out that energy absorbed in the infrared spectrum is associated with the excitation of vibrational states and in the microwave spectrum with rotational states of the atom or molecule. Given the empirical model of the atom, in order to know whether a particular absorption or emission is possible, we need to determine the quantum 'transition probability' from the overlap of the initial state, photon state, and final state. If this is non-zero, it is possible. But, as in the case of chemical bonding, for the mathematical overlap function to be non-zero certain relationships between the symmetries of the states must hold.

A more dramatic example is provided by the deductive argument associated with the discovery of quasicrystals in 1984. Crystals had been regarded as periodic structures composed of space-filling building blocks. By then the range of possible symmetries of crystals was well known; in particular it was known from the 'Crystallographic Restriction Theorem' that fivefold symmetry is mathematically impossible. A crystal cannot have fivefold symmetry because a unit cell with fivefold symmetry (like the dodecahedron beloved of Plato) cannot be stacked up to completely fill space — gaps will form between cells. So when a crystal that was a novel species of an alloy was shown, by X-ray diffraction techniques, to exhibit fivefold symmetry it generated the same kind of "intellectual shock" that Mach described as the response to the Ørsted experiment. Because the mathematics could not be wrong and the deductive argument was valid, the feeling was that Nature had somehow defied the principles of logic. But there's no mystery about any symmetry *inference* here. What was (unexpectedly) wrong with the argument as a whole concerned an implicit premise that was used with a normal deductive inference. That faulty premise was that the substance was actually a crystal in the special sense of having a periodic structure. Alloys of the type investigated *seem* to be crystals because their regular space-filling structures display symmetries and give rise to other crystal-like properties. But they are unlike crystals in other ways: their space-filling structures involve two and sometimes more types of unit cell and those cells are stacked aperiodically. This was all rather new and surprising — so new in fact that even the mathematics of aperiodic tiling, the two-dimensional analogue of these structures, had not been generally known before the 1970s.

Deductive inferences are not symmetry inferences, even when they are applied to premises that happen to refer to symmetry, because they do not depend for their validity on the concept of symmetry or on any other non-logical concept in the propositions to which they are applied.

Abductive Inferences

A scientific inquiry typically starts with abduction, a conjecture about what explains some otherwise surprising observations from which they would then follow as a natural consequence. The conjecture can then be used as a premise for a forward-direction deductive argument that yields testable predictions.

Consider the example of abductively inferred symmetries of internal structure. Woldemar Voigt (1850-1919) suggested in 1887, on the basis of crystallographic studies that he and others had undertaken, that one could start with observations of the form of a crystal and then abductively infer what are, in effect, its internal structural symmetries. These inferred symmetries would then be the basis for deductive inferences about various other properties, such as elastic behavior, the conduction of heat, and the propagation of light. As he says:

> Observations have shown that in all known physical properties (e.g., with respect to light and heat) crystals possess at least the symmetry of their form, and in most cases still higher symmetries. Therefore, it seems appropriate to [infer] from the crystalline form the most general law of symmetry of the crystalline substance, and to assume that the crystal displays the law including the symmetries in all physical properties. (Voigt qtd. in Katzir, *Piezoelectricity* 79)

In other words, the symmetry of the internal structure is a scientific hypothesis that goes beyond what would be expected to follow from the external form alone; it has 'excess empirical content'- in that it can be used to make novel, testable predictions. Like all hypotheses, an initially posited symmetry may need to be modified to improve agreement with further observations, such as when we press it to make predictions about physical properties other than the ones from which it was abductively inferred.

Abductive inferences are not formally valid; their conclusions (which are conjectures) are not certain but can be corroborated or challenged by empirical testing. One problem is that hypotheses are underdetermined by empirical data. For abductive inferences — not just those concerned with symmetry — it would be useful to have a principled way to choose among the various conjectures compatible with the data.

Inductive Inferences

Inductive inferences also use particular observations to support general conclusions. Unlike abductive inferences, these general conclusions are generalizations about particular observations rather than explanations of them. Inductive inferences are neither valid nor invalid; they are just strong to some degree. Their conclusions are never certain, just probable to some extent.

I illustrate induction by Pasteur's famous claim in 1860 that associated asymmetry in crystal form with living processes and associated both asymmetry and living processes with optical activity, the capacity of a compound in solution to rotate the plane of polarization of light passing through it. Other scientists

had already drawn attention to evidence that many natural substances — for example, camphor, sugars, oils, oil of turpentine, nicotine, and above all tartaric acid itself — displayed optical activity in solution, while no inorganic substance had been found to possess this property when dissolved. (Geison, *Private Science* 101)

Pasteur then added the results of his own experiments on tartaric acid and amyl alcohol. By that time, a small number of particular observations had shown that:

- Some chemical compounds crystallized in two asymmetrical forms that were mirror images of each other.
- Production of these compounds by artificial (i.e., non-living) processes resulted in equal quantities of both forms.
- Production of these compounds by living processes resulted in only one form.
- If one wants a sample that contains only one crystal form, one could produce it

naturally from a living process or, as Pasteur did, by manually segregating the crystals resulting from the mixture that an artificial process produces.

- Solutions of compounds comprising only one crystal form are optically active; those containing both forms in equal quantities are not.

Pasteur took an inductive leap. “Pasteur,” Geison claims, “very swiftly extended the more limited claims … into a fundamental division of the natural world into optically active and optically inactive substances” (*Private Science* 101). It was his work on tartaric acid in particular that suggested to Pasteur that nature created optically active substances by favoring only one of a pair of symmetric alternative crystal forms for the product. Pasteur claimed that

> optical activity and life are somehow intimately associated, and the production of a single optically active substance unaccompanied by its mirror image is indeed nature’s prerogative except under highly exceptional and basically “asymmetrical” conditions. (Pasteur, qtd. in Geison, “Louis Pasteur,” 361)

Pasteur’s claim is based on an implicit inductive symmetry inference. To make the inductive core of the argument clear, and to highlight why this example will challenge any purely formal account of the argument’s strength, I need to make some of the complicating details explicit.

- There are at least two arguments here — one connecting living processes to asymmetric mixtures of molecules, the other connecting that asymmetry to optical activity. Let’s simplify by focusing on the symmetry inference, which I paraphrase as:

“Only living processes can produce asymmetric mixtures of molecules.”

- Since only some living processes lead to asymmetry, the universal claim that is most obviously a candidate for inductive support is the one expressed as the negative of the original claim. That claim is:

> Each non-living chemical process yields a symmetric mixture of molecules.
>
> Therefore, by induction, all non-living chemical processes yield symmetric mixtures of molecules.

Expressed this way, the claim now seems uninformative; it was clearly the surprising fact that living processes often yielded asymmetric molecules that begged explanation.

- In any case, this universal claim is inductively supported by very few particular cases, namely the handful of chemicals that Curie and others before him had investigated. The inference would be very weak if it had to be warranted by the number of confirming cases.
- Even then the argument is protected by the phrase “except under highly exceptional or basically ‘asymmetrical’ conditions,” on the face of it a question-begging move. Pasteur makes it clear elsewhere that he does not want to include in the class of ‘non-living processes’ any artificial ones that use biological feedstock as this could already consist of asymmetrical mixtures of molecules — industrial fermentation, for example.

> When I affirm that no artificial substance has yet presented molecular [asymmetry], I mean to speak of artificial substances, properly so called,

> formed entirely of mineral elements or derived from non-[asymmetric] bodies. (Pasteur 21)

This is actually a very reasonable restriction, but one that can be further specified in a non-arbitrary way using background knowledge of the science.

Pasteur's conclusions have since been highly corroborated and are generally accepted today, so it is worth reflecting on what warrants his induction. The upshot of this brief description of his claim is that it will be hard to gauge the strength of the inductive argument without significant recourse to background information about the theories and practices of the science concerned — or even to cleanly characterize the argument as an induction at all.

2.2 The Material Logic of Symmetry

I noted above that inferences that are necessarily valid in virtue of their form cannot, for that reason, be specific either to a symmetry concept or to any particular domain of use or discourse. Therefore to determine how considerations of symmetry itself warrant inferences we need to focus on non-deductive inferences. But regardless of how we classify these non-deductive inferences (e.g., as 'abductive' vs. 'inductive' or as being specific to some part of the process of scientific inquiry) we will still need a way to recognize which of them are warranted and which are not.

One conceivable approach to finding warrants for such inferences would be to seek universal rules that make no reference to any particular domain of use or discourse. Although any such rules would govern hypothetical or probabilistic inferences, they would nevertheless be formal and *a priori*. The quest for such schemas though has proved fruitless for both induction and abduction. Despite a vast literature, there is no purely formal solution to 'the problem of induction,' in either its Humean or modern form. (See Norton, "A Material Dissolution of the Problem of Induction.") Nor is there any formal 'logic of discovery,' i.e., no formal solution to the problem of abduction either.

Another, more promising, approach to finding warrants for inference is to seek rules that are specific to a particular domain of use or discourse. Peirce, around 1885, identified this approach and called it 'material logic':

> Formal logic classifies arguments by producing forms in which, the letters of the alphabet being replaced by any terms whatever, the result will be a valid, probable, or sophistic argument, as the case may be; material logic is a logic which does not produce such perfectly general forms, but considers a logical universe having peculiar properties. (CP 2.549)

Dewey added that such domain-specific rules cannot be *a priori* but would themselves part of the inquiry:

> [A]ll logical forms (with their characteristic properties) arise within the operation of inquiry and are concerned with the control of inquiry so that it may yield warranted assertions. (*Logic* 3-4)

Material logic in this sense could be conceived either as a set of formally valid inferences with missing material premises (i.e., as enthymemes) or as a set of material rules of inference. Enthymemes would seemingly make an attractive basis for material logic on the grounds of simplicity because no additional forms of inference would have to be entertained. But Wilfrid Sellars argued that one need not interpret material logic this way. He analyzed six alternate conceptions of the status of material inferences, and concluded that material inference itself is as essential to meaning as formal inference because "there are an indefinite number of possible conceptual structures (languages) or systems of formal and material rules, each one of which can be regarded as a candidate …" (337). Furthermore, these candidate schemes would have to compete in "the market place of practice" (337). That is, there is no unique system of logical and material inferences and concepts that one can know *a priori*; one discovers the combination that in practice works best.

Concepts, correlatively, would also be discovered empirically in "the market place of practice" as part of the combination of concepts and inferential rules that provides the best empirical account of phenomena. Robert Brandom develops this principle of Sellars to base his theory of concepts not on some origin in human experience but on the inferential roles they play.

> The kind of inference whose correctnesses determine the conceptual contents of its premises and conclusions may be called, following Sellars, material inferences. (*Reasons* 52)

If we follow Brandom, we can thereby make the various scientific concepts of symmetry explicit by determining the roles those concepts play in scientific inferences.

Concepts are based in the inferential practices of inquiry and for that reason are historically situated as well. "Grasping a concept is mastering the use of a word—and uses of words are a paradigm of the sort of thing that must be understood historically"

(Brandom, *Reasons* 27). Concepts (and the inferences that imbue them with meaning) will also have a history. An appropriate historical epistemology would make that history explicit and explain the mechanisms driving historical change and I seek to use one to elucidate the warrants for symmetry inference.[4]

2.3 The Material Warrants for Symmetry Inference

We have demanded the warrants for material inference based on symmetry, so it is important to understand what kind of an account of symmetry would constitute a satisfactory response. We ask for warrants because we find it surprising how effective symmetry arguments have been in the physical sciences despite the fact that their validity cannot demonstrated on formal grounds. Offering synonyms for ‘warrant’ would not be a useful response; we are not asking for a paraphrase of the original argument but a reason to feel confident about the overall process.

The early American pragmatist philosophers Peirce and Dewey hint that the response we are seeking is a confidence-building explanation rooted in the nature of inquiry, the general systems and processes that are applied to making specific material inferences. In the spirit of Peirce the warrant we seek for symmetry inferences would be an “an explanatory hypothesis” for the “surprising fact” that symmetry arguments are so successful — which he would take to mean that such a warrant can only be conjectured if its truth would make that success “a matter of course” (CP 5.188-189). In the spirit of Dewey, symmetry inferences would have ‘warranted assertability’ insofar as they were

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[4] Ingo Brigandt shows in “Scientific Reasoning” that all scientific reasoning is material inference, which is consistent with the position I take in the analysis.

made in the context of on-going and self-correcting processes of inquiry.

> The distinction between true and false conclusions is determined by the character of the operational procedures through which propositions about data and propositions about inferential elements (meanings, ideas, hypotheses) are instituted ("Warranted Assertability" 176).

Following their lead, our task is to provide a deflationary account of scientific inquiry, one where the conclusions of symmetry arguments, while admittedly fallible, are nevertheless warranted whenever they follow 'as a matter of course' from generally reliable procedures. The general success of symmetry arguments would no longer remain 'surprising' nor the occasional lack of empirical corroboration 'shocking.' Conceived this way, the task is not to further analyze symmetry definitions, concepts, and propositions in the hope of ferreting out hidden premises or any other logical connectives that would legitimize the symmetry arguments, but instead to provide a convincing account of the historical and fallible processes of empirical inquiry and of the material context in which symmetry concepts arose, developed, and were successfully deployed.

The specific type of symmetry warrant we seek will depend on the type of surprise it alleviates. I distinguish three types so that we can see later whether the historical epistemology we employ will address factors that are relevant to determining whether such warrants exist and how they operate.

Projectable Warrant

Concerning a given research program at any one time, we might wonder why symmetry arguments keep generating conclusions that are then empirically corroborated.

What is surprising is that the particular concept of symmetry we are using is projectable, that is, extendable to instances beyond any that might have been used to posit the symmetry in the first place. For example, what is it about geometric notions of symmetry that make them so suitable for classifying the external forms of crystals or predicting their physical properties? What I call the projectable warrant is the explanation for the continued success of repeated applications of what is recognizably the same inferential practice within a research program at a given stage of its development.[5]

Evolvable Warrant

Concerning a given field but over time, we might wonder why symmetry, broadly conceived, can continue to be reconfigured to restore projectability in response to an empirical challenge (newly discovered phenomena or increased precision in measurements, say). Extending the previous example, how has symmetry been able to morph from (say) a geometric to an algebraic concept in crystallography? Are these concepts variants of the some more basic concept of symmetry? If so, how likely is it that future variants will arise in response further empirical challenges as well? What I call the evolvable warrant is the explanation for our continued success in developing new projectable warrants on the basis of concepts that are recognizably variants of earlier

[5] A biological analogue of symmetry warrant in this sense is an understanding of the fitness of a population in an environmental niche.

concepts of symmetry.[6]

Transferable Warrant

Finally, we might wonder how symmetry inferences honed in one domain can be transferred for use in another. We know that since the time of Pierre Curie, if not before, they have been. Curie showed that symmetry inferences used in crystallography can be used in electromagnetism and other physical domains. What I call the transferable warrant is the explanation for successful transfers of symmetry reasoning from one domain to another.[7]

2.4 Example of a Projectable Warrant: Pasteur's Claim

Having excluded deductive inference for the reasons given earlier, I will seek inferential warrants only for material inferences. There are no formal criteria for validity for such inferences; instead we need to regard their inferential strength as dependent on context and content.

I illustrate this with Pasteur's claim associating asymmetry, life, and optical activity. I briefly described this inference above and noted there the difficulty in providing a warrant that was formal as opposed to material. I now argue specifically why

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6 A biological analogue of this warrant is an understanding of the continuing adaptability (at least thus far) of a species, through variation and natural selection, to respond to the demands of a changing environment.

7 The biological analogue here is the more abstract notion of an adaptive trait, which, if genetically accessible to any species or population, would facilitate its survival and reproduction in some given environment.

Pasteur's claim should be regarded as a material one and warranted accordingly.

At the time Pasteur made his claim, it was supported neither by a large mass of data nor by any formal inductive schema, such as sampling techniques. The credibility of his claim continued to increase, but not just because further case material of the same sort was amassed nor because there was any critical breakthrough in formal methods of inductive analysis. Rather, his claim seemed to draw strength from the advances in experimental technique, instrumentation, and empirical knowledge. This suggests that, if we are able to warrant it all, we need to regard the claim as the outcome of a *material* induction, one grounded in facts known in Pasteur's day, even though those facts hold only in restricted domains — such as symmetry in the domain of crystallography, optical activity in physics, and so on.

Certain features of Pasteur's inquiry provide evidence that his claim was indeed based on a material inference and, as will become apparent, these features show how the warrant arises. This evidence can be found by comparing the historical development of his ideas (recounted in many places, for example, in cited works by Geison, Benninga, and Katzir) with the features that Dewey identified as characteristic of a material logic (*Logic* Chapter XXI).

One such feature is the presence of a problem context. The context in Pasteur's case was the spectacular advance organic chemistry between 1820 and 1860, the period in which Pasteur was working. Unlike inorganic chemistry, which covers a large number of elements combined in simple proportions, organic chemistry focuses primarily on a small number of elements (carbon, hydrogen, oxygen, and, to some extent, nitrogen and trace elements) combined in a vast number of ways. Many different organic compounds are composed of the same elements in the same proportion. To make sense of that, chemical formulas had been adopted to represent not only the proportions of chemical elements in the compound but also their structural arrangement, so that different compounds with the same composition (i.e., the same chemical proportions) could at least be distinguished by their structures. The atomic theory was still controversial in the nineteenth century, and although it was not the only way to make sense the proliferation of organic compounds and their reaction paths, those favoring this theory certainly regarded these structural formulas as literal maps of the atoms in a molecule of the compound and the posited arrangements as ways to explain the various reaction paths of those compounds. But the emerging problem situation for this developing science was this: in 1844 Eilhard Mitscherlich had found an apparent exception. It seemed that the sodium-ammonium salts of paratartaric acid and tartaric acid had both the same formula (composition) and the same crystal form (structure) *yet still differed*. They differed in at least this remarkable way: solutions of the tartrate were optically active, rotating the polarization of light to the right, while solutions of the paratartrate were not optically active at all. This was obviously a problem because it was not clear what other than composition and structure could possibly account for this difference in properties. Jean-Baptiste Biot (1774 - 1862), the undisputed expert in optical activity, referred this problem to Pasteur in 1847.

A second feature is that the problem is not constituted by immediately given observations (as it seems to be in some paradigm inductions about sunrises, white swans, white powders, etc.). Rather, according to Dewey, the problem itself “can be defined here only in terms of the operations of transforming antecedently given material of perception into prepared material” (*Logic* 432). This characteristic of material logic is present in the inductive phase of a scientific inquiry. In our example, we see the that problem of optical activity that Biot bequeathed to Pasteur could not be constituted by immediately given observations simply because specially constructed scientific instruments were needed to observe optical activity — indeed this had not been done until Biot himself discovered the phenomenon in 1812. We also see the given material (the crystals anyone can see) were transformed into material prepared according to the categories (such as crystal forms) in which Pasteur was already keenly interested for other reasons. Admittedly, if crystallization is done very carefully and if the crystals are large enough, crystal form is immediately given to the naked eye. But this would not have been good enough for Pasteur’s purposes. Pasteur needed to prepare his material to make it amenable to his more sophisticated investigation. He had already noticed something that others had missed. While the crystal forms of the paratartrates are the same as those of the tartrates (both are an asymmetrical shape classed as ‘hemihedral’), paratartrates are actually a 50:50 *mixture* of two variants of that asymmetrical structure. One variant has hemihedral facets on the right-hand edge, and are identical to those of the tartrate, while the other had hemihedral facets on the left-hand edge. The latter type are not represented in the tartrate sample. Pasteur was interested in that distinction and so he prepared the sample of material so that it had evidential weight for his inductive generalization. Pasteur, a consummate experimentalist with a background in crystallography, used a pair of tweezers to very carefully separate the two mirror-image crystals of the paratartrate. Then, in the presence of Biot, showed that the solution of the right-faceted crystals rotated the polarization of light to the right, as the tartrate did, that a solution of the 50:50 paratartrate mixture had no effect, and that the solution of the left-faceted hemihedral crystals rotated polarization to the left. The latter was a predicted effect that could not have been witnessed until the material had been transformed to provide this new data of the relevant kind.

A third feature of Pasteur's is the determination of identities and differences. According to Dewey, "scientific inquiries search out relevant data for their problems by means of experimental determination of identities and differences" (*Logic* 426). By 1848, through the above experiments, Pasteur was able to provide a complete solution to the problem that Biot had posed by introducing a new identity, namely symmetry, and by distinguishing ways in which this newly introduced concept was to be applied. First, an *individual* crystal would be regarded as symmetric (or, more accurately, as bilaterally symmetric) if it could be superimposed exactly on a mirror image of itself. A perfect cube is symmetric in this sense. Objects that are not symmetric in this way (one's right hand, for example) are now referred to as 'chiral.' Second, a *pair* of asymmetric objects would be bilaterally symmetric if they comprised a matched pair of chiral objects, i.e., a pair in which each was the mirror image of the other. The right and left hands are (approximately) symmetric in this second sense. So by then it seemed reasonable to infer an association of two observational variables: optical activity and asymmetry, *viz*. that asymmetry (of the crystal form of an organic compound, unmixed with its chiral opposite) was associated with optical activity (of a solution of that compound). This inference was then further strengthened not only by the addition of new conforming cases but also by his eventual exclusion of a rival theory concerning structure.

A fourth feature is problem selection. Pasteur's second big breakthrough, the one that concerned fermentation, illustrates Dewey's idea of the way "[p]articulars are *selectively* discriminated so as to determine a *problem* whose nature is such as to indicate possible modes of solution" (*Logic* 424). In this case, the particular optically active substance that Pasteur selected to continue his studies was amyl alcohol. This substance was not added just to strengthen the induction by boosting the number of cases, as one would expect if inductive strength could be quantified in a purely formal way. Rather, he discriminated among the particulars, and this compound had special significance in the problem context. If one were writing an 'external history' of this work, one could point to the problem of the brewing industry in Lille, where Pasteur was working, since amyl alcohol is a by-product of alcoholic fermentation and a local distillery had asked him for help. But in his own writings Pasteur describes the choice of amyl alcohol as following the 'internal logic' of his research. He had discovered two forms that had the same chemical composition, one of which was optically active. There are in fact a large number of optically active compounds that result from fermentation, but what piqued his interest in the amyl alcohols in particular was that they constituted the first exception to a rival inference, his earlier inductive inference that optical activity was correlated with form, specifically hemihedral form (Geison, "From" 95). From these and other studies of fermentation over the following decade, Pasteur became convinced of the correlation between asymmetry and living processes. By 1860 he presented his bold conclusions to the Chemical Society of Paris (Pasteur 1-32).

We should also note that Pasteur's material reasoning had general support from the allied domain of crystallography, in which he was also well versed. In that field it was already generally accepted that crystal form, and therefore its symmetries, were determinant of the physical properties of crystals as well as of molecular shape. Although the atomic hypothesis was still controversial in the nineteenth century, Pasteur himself accepted that crystal form was somehow related to molecular structure and thus it would have been very reasonable to expect that any asymmetries in crystals would be reflected at the molecular level, where a mechanism for molecular interactions with light would one day explain optical activity. His induction gave him a useful proxy for substances associated with living processes, namely asymmetry, which could be determined by optical activity, a far less tedious way than separation and classification of crystals. Fermentation, he argued, was a due to a living microorganism because its products were asymmetric.

There is much more that can be said about Pasteur's argument, including the way he refined and advanced the concept of symmetry to meet his inferential needs, but this should suffice for now to suggest that it is no more likely there will be a universal schema for inductive symmetry inferences than that there will be a universal logic of discovery for all abductive symmetry inferences. If neither of these is universal, how then can one say anything at all about their warrants?

The characteristics of material logic, illustrated above using Pasteur's inquiries, suggest that inferential warrants arise and develop through the mutual accommodation of the various phases of scientific inquiry. The scientific process is a historical one: cases may be selected for investigation because they seem capable of adjudicating between current rival models, like those based on the concept of form and those based on the concept of symmetry. New experimental techniques may identify phenomena not previously observed, like optical activity, and transform objects of study into prepared material, like samples of crystals with different previously unrecognized differences in symmetry, and so on. The science and the concepts used to make scientific inferences are tested and adopted as a package.

2.5 Examples of Evolvable Warrants: Science, Mathematics, and Symmetry

Evolvable warrants, by contrast, apply to conceptual adaptations over time. What warrant justifies our continued reliance on modifications to the symmetry concept so as to maintain the reliability of inferential practices? I illustrate what is meant by evolvable warrants through recent efforts to use conceptual adaptations as warrants in science and mathematics more broadly. The first question is: What explains the 'miraculous' success of science? The second is: What explains the 'unreasonable' effectiveness of mathematics in science? By parallel reasoning, I posit an answer about symmetry that I will develop more fully in the case study.

The 'Miraculous' Success of Science

One parallel concerns the evolvable warrant for science itself. The 'miraculous' success of science parallels the 'surprising' utility of the symmetry concept and so it is worth looking at the proposed warrants for that success. Karl Popper claimed that the ‘miraculous’ success of science could not be explained at all (204). But, subsequently, many arguments have been put forward in an endeavor to explain that success. Hilary Putnam, for example, famously suggested that scientific realism was “the only philosophy that doesn’t make the success of science a miracle” (73). My concern here is not with scientific realism or even with how miraculous the success of science actually is but only with the types of warrants that have been suggested.

Dewey already left us with the idea that the ‘warranted assertability’ of propositions arose out of the processes of the inquiry used to generate them rather than out of an analysis of logical form or conceptual content alone. Those processes are historical and fallible so that leaves us with the question of explaining why any set of processes provides ‘true’ answers.

Bas van Fraassen in effect solves that issue of truth by reliability, claiming that scientific theories (and, by extension, symmetry inferences) can be reliable without representing anything ‘real.’ Although he does not need to deny truth, it is sufficient for his purposes that the theory is empirically adequate, i.e., that it describes actual and potential observations in a self-consistent way. We can feel confident that these theories will be reliable because unreliable ones will be weeded out. Van Fraassen gives a Darwinian account of the success of science as follows:

> I can best make the point by contrasting two accounts of the mouse who runs from its enemy, the cat. St. Augustine already remarked on this phenomenon, and provided an intentional explanation: the mouse perceives that the cat is its enemy, hence the mouse runs. What is

> postulated here is the 'adequacy' of the mouse’s thought to the order of nature: the relation of enmity is correctly reflected in his mind. But the Darwinist says: Do not ask why the mouse runs from its enemy. Species which did not cope with their natural enemies no longer exist. That is why there are only ones who do. (*Scientific Image* 39)

He continues:

> In just the same way, I claim that the success of current scientific theories is no miracle. It is not even surprising to the scientific (Darwinist) mind. For any scientific theory is born into a life of fierce competition, a jungle red in tooth and claw. Only the successful theories survive — the ones which in fact latched on to actual regularities in nature. (Scientific Image 40)

This of course requires that the scheme we use to account for theories or symmetry inferences can at least accommodate rival theories, since there is no selection without alternatives. Brad Wray lauds van Fraassen’s approach as superior to realist explanations of science’s success because it also “provides us with resources to adequately explain the failure of past successful theories and the fact that successes can be shared by two competing theories” (88-89). But it still leaves us with the question about predictions, of why empirically adequate theories and symmetry inferences should be expected to continue adapting to new circumstances.

Ian Hacking, although not part of the conversation on van Fraassen’s views, provides a way out. Theories and symmetry inferences would be, if I can be permitted to extend van Fraassen's imagery, more like ecosystems than mice. In Hacking's approach, the warrant for the theory or symmetry inference comes from *mutual* adaptation of concepts, theories and experimental practices — a process he terms 'self-vindication' ("Self-Vindication" 53). If we were to use a biological metaphor, it would not be van Fraassen's image of an organism waiting for mutations to occur but an image of organisms not only responding to each other, to other organisms, and to their environment but also (like humans) shaping it. Theories and symmetry inferences would be far more robust under these conditions and more capable of making predictions. That still leaves us with a challenge, albeit a focused one, to be taken up in the development of a historical epistemology: What is the mechanism by which all those components mutually adapt?

If the warrants of symmetry arguments were at all like this, we would need to give an account of them in terms of conceptual co-adaptation, more or less along the following lines:

- Inferential warrants of symmetry are to be found in the fallible, historical processes of scientific inquiry, not in conceptual or logical analysis (Dewey).
- Those processes lead to reliable patterns of symmetry inference because they out-compete rival patterns (van Fraassen) and because adaptation is mutual, involving not just the concepts of symmetry but also other conditions, such as experimental interpretations and practice, scientific theorizing, and mathematics (Hacking).
- There are specific mechanisms that drive that adaptation.

The 'Unreasonable' Effectiveness of Mathematics

A second parallel concerns the evolvable warrant for the use of mathematics. In his celebrated 1959 essay, "The Unreasonable Effectiveness of Mathematics in the Natural Sciences," Eugene Wigner (1902-1995) identifies a "mystery" that could easily be rephrased to express astonishment about the degree of success that symmetry inferences have. Wigner makes the point

> that the enormous usefulness of mathematics in the natural sciences is something bordering on the mysterious and that there is no rational explanation for it. (223)

If by "rational" Wigner implies "*a priori*" that need not trouble us too much; symmetry inferences are material and *a posteriori* warrants would be enough to boost our confidence in them.

To help dispel that mystery about effectiveness one can usefully recast the problem as a pragmatic one about the applicability of mathematics. Rather than vainly hoping to demonstrate rationally that mathematical reasoning is valid or that mathematical concepts refer to something real, one would instead try to show empirically how its structures are selectively developed to describe what is known about the world. In this vein, Mark Steiner notes two problems with Wigner's "mystery," namely that

> [Wigner] ignores the failures, i.e., the instances in which scientists fail to find appropriate mathematical descriptions of natural phenomena (which outnumber the successes by far). He also ignores the mathematical concepts that never have found an application. (9)

Steiner also notes that mathematics sometimes provides the very framework in which we posit new laws (4) — at least in fundamental physics, where our common sense stock of analogies and metaphors no longer serves this purpose. Likewise, Steven French claims that “this effectiveness can be seen to be not so unreasonable if attention is paid to the various idealising moves undertaken” (103), such moves being the ones needed to represent the real world in a way that makes the mathematics either tractable or applicable at all. French also makes use of the history of the relationship between mathematical structures and the structures of the scientific theories it supports in order to illustrate the role of conceptual co-adaptation in bringing about this effectiveness.

Conceptual adaptation may well dispel some of the mystery about symmetry inference as well. French illustrates the effect of co-adaptation in the context of the introduction of the mathematics of group theory, which is the language of symmetry, into the science of quantum mechanics. As he notes, this is a good case to propose for historical study because it treats new mathematics and new physics, both of which we can observe, as it were, in real time — unlike the case of calculus and Newtonian mechanics which is more than 300 years old. It also meets Wigner on his home turf. Among other matters, French observes that

> both group theory and quantum mechanics were in a state of flux at the time they were brought into contact and both subsequently underwent further development. The structures may therefore be regarded as significantly open in various dimensions … (110)

French again notes a number of “idealising moves,” in this case study, such as deeming certain particle properties to be equal when they were known to be only approximately so in order to make the formalism work. Embedding a scientific theory into a mathematical structure essentially benefits the theory by giving it access to the surplus inferential capacity of the mathematics, which aids the theory's further development (104).

The 'Surprising' Utility of the Symmetry Concept

Our issue is the evolvable warrant for symmetry. If we follow the spirit of the pragmatist philosopher Peirce, a warrant for a symmetry inference would explain its success, making it no longer 'surprising' but something that happens more or less as 'a matter of course.' Although we don't expect to do so using *a priori* reasoning, we may be able to reduce the surprise by revealing the mechanisms by which the concept of symmetry and its mathematical language have adapted to the changing inferential needs of the sciences that symmetry supports.

3. THE HISTORICAL DEVELOPMENT OF SYMMETRY

In Chapter 1 I identified several senses in which symmetry is commonly understood and in Chapter 2 I illustrated some of the many material inferences that have been based on symmetry. In this third chapter I consider how best to provide an account of the warrants for symmetry inferences.

3.1 Inferential Practices

Inquiry comprises practices, and so we need to study the inferential practices involving symmetry. To root any warrant for symmetry inferences not in logic but in these practices of inquiry, we can seek guidance in the studies of scientific practice that have been undertaken in the last 30 years or so, following the 'practical turn' in the philosophy of science. "[T]he key advance made by science studies in the 1980s," according to Andrew Pickering, in the introduction to his compendium *Science as Practice and Culture*, "is the move toward studying scientific practice, what scientists actually do …" (2). Ian Hacking had revived this focus on practice in 1983 in response to what he saw as a crisis of rationality in science that followed in the wake of Thomas Kuhn's characterization of scientific change; Hacking moved "to a simpler, more old-fashioned concept of history, a history not of what we think but of what we do" (*Representing* 17). If we were to follow this historiographical program in regard to symmetry we would seek an understanding of changes in and applications of symmetry concepts and principles — not in some deeper theory but in empirically validated inferential practices. This in fact was the approach that Lorraine Daston and Peter Galison take in their magisterial 2007 study on objectivity — which they term a "nebulous notion." (Like symmetry perhaps?) They treat objectivity not as a concept but as a practice (perhaps even as an epistemic virtue) and claim that, "if actions are substituted for concepts and practices for meanings, the focus on the nebulous notion of objectivity sharpens" (52).

Inferential practices involving symmetry, like all practices, are always historically situated, and so we need to account for them historically. That is, we need to do more than just study inferential practices; we need to study those practices as depending on symmetry and as specific to a scientific field at a particular period in its development because, as concepts change and as the needs of inquiry vary from time to time, so too do inferential practices.

We already know *that* the concept of symmetry has changed from time to time, since there have been several histories of the concept. While most of the literature on symmetry is technical (covering specific scientific or mathematical applications or treating particular philosophical issues) there are some long-view historical surveys. None self-consciously adopts any particular historiographical methodology, and all freely refer to both external factors and to the internal logic of symmetry in the narration. They have different emphases and on specific matters sometimes come to different conclusions.[8]

[8] See, for example: Du Sautoy; Hon and Goldstein, 2008; Selzer; and Stewart.

We also need to know *why* the concept of symmetry has changed, since the variations in symmetry's meaning that are recorded in those histories may have been due to something other than changing inferential demands. Those histories differ, not because one is 'right' and the others 'wrong,' but just because they represent a healthy plurality of aims and interests. For my project, it therefore behooves me to narrate the history of symmetry in a way that recognizes the epistemological nature of both science and symmetry. Hans-Jörg Rheinberger notes in his influential survey of this issue that various ways to do this (i.e., to historicize epistemology) have already been articulated; he claims, further, "the historicization of epistemology represents a decisive moment in the transformation of twentieth-century philosophy of science" (1). One way to understand historicized epistemology is as the study of "higher-order epistemic concepts such as objectivity, observation, experimentation, or probability" (Feest and Sturm 285), a list which could presumably be expanded to include symmetry.[9]

I propose to study the concept of symmetry, and the inferential practices involving it, using a historical epistemology guided by best practice. As the historically situated practices are contingent I need to study them *a posteriori* using historical case material.

3.2 Historical Case Studies of Symmetry Inferences

Historical case studies can be selected in many ways. The scientific field, programs, and era are neither unique nor pre-determined in any way; they will depend on, among

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[9] The authors acknowledge pluralism. Two other major categories of historicized epistemology include those of 'epistemic things' (exemplified in the work of Hans-Jörg Rheinberger) and long-term scientific developments (exemplified in that of Jürgen Renn).

other things, the research question, the epistemic objects to be tracked, and the plausible rival claims we wish to evaluate.

My own chosen focus is on the co-adaptation of the symmetry concept in modern science, the tracking of symmetry inferences, and the evaluation of identified rival claims (co-adaptation and non co-adaptation). It is widely believed that symmetry arguments emerged in crystallography in the nineteenth century and from there spread into the physical sciences. In the Prologue, I began with the view like this expressed by the renowned physicist and crystallographer, Pierre Curie. He is in fact widely credited in the physics community for formally initiating that transfer in his influential 1894 paper, "On the Symmetry of Physical Phenomena, Symmetry of an Electric Field and of a Magnetic Field." He began by announcing his goal: "I think that there is interest in introducing into the study of physical phenomena the symmetry arguments familiar to crystallographers" (17), implicitly claiming that crystallography was what could be called the 'native domain' for symmetry inferences and that these inference forms could be transferred to various subfields of physics. A century later, that was still the dominant view. Shlomo Sternberg, a mathematician, acknowledged those particular empirical origins this way:

> Symmetry considerations entered into the solutions of physical problems at the very beginning of mathematical physics. Mathematical crystallography, a major success of 19th century physics, is essentially group theoretical, but it had developed before the abstract language of group theory had been accepted. (x)

This is hardly surprising, since, to use Barding and Castellani's phrasing,

> [t]he natural objects with the richest and most evident symmetry properties are undoubtedly crystals, and so it is not surprising that the systematic study of all possible symmetric configurations — the so-called theory of symmetry — started in connection with the rise of crystallography. (4)

I will provide a material account of the symmetry warrant based on the idea of co-adaptation in the very promising historical setting of nineteenth-century crystallography. I will also critically examine *non* co-adaptation claims that symmetry concepts arose independently in mathematics and only later found application in the sciences (§4.5).

We should encourage a pluralist approach to these case studies. One reason of course is that we might be wrong and should fairly consider rival claims. A second reason is that we can also enrich our understanding by pursuing *non*-rival claims, claims that just target different questions. Yet a third is that we can sometimes recover valuable knowledge even from defunct scientific research programs. This will become apparent in the case study in Chapter 4. The scientific theories in which symmetry inferences were embedded in the early nineteenth century (namely, the French molecular theory and German polar theory) are no longer held. Furthermore, it was sometimes possible to make important *symmetry* inferences about phenomena (such as pyroelectricity and piezoelectricity) even though there is no underlying theory about the phenomena at all.

3.3 Historical Epistemology

Each type of case study will require its own approach. We may call such approaches historical epistemologies, understood in Rheinberger' s sense as

> reflecting on the historical conditions under which, and the means with which, things are made into objects of knowledge. It focuses thus on the process of generating scientific knowledge and the ways in which it is initiated and maintained. (2-3)

Feest and Sturm offer a useful (although non-exhaustive) taxonomy of such epistemologies according to the nature of the inquiry.

Among the plurality of historical epistemologies, the type that would cover the historical development of symmetry is the history of an epistemic concept. Feest and Sturm understood this type more specifically as covering "the history of higher-order epistemic concepts such as objectivity, observation, experimentation, or probability" (285).

Although the nature of 'the history of an epistemic concept' is not articulated in any formal schema, the literature on and paradigmatic examples of historical epistemologies of this sort — especially those about concepts closely related to symmetry — mark out some basic features that would be important for a conceptual history of symmetry; for example:

- Practices can identify concepts. We see this in Ian Hacking's *The Emergence of Probability*, one of the earliest works in this genre, which traces the concept of probability in its several senses through connections with inferential practices in various walks of life.
- Conditions of identity can allow us to say of a concept that it actually has a history. In other words, it's not always a matter of one concept just replacing an earlier one but

sometimes of a concept that changes while still maintaining a continuity with its past (Feest 290).

- Identifiable mechanisms can explain conceptual change (or, alternatively, conceptual stability). We need not presuppose any mechanism at the outset, but should remain alert to historical evidence for any such mechanisms. For example, if inquiry is self-correcting, how were success and failure recognized in research programs? Under what circumstances was conceptual change regarded as a remedy for failure?

3.4 Narrating a Historical Epistemology of Symmetry

Histories are many for the same reasons that maps are many: they address different questions. We need to be selective therefore, but not tendentious, and to highlight features that are relevant, one way or another, to the question posed. I propose therefore to narrate the case study offered in Chapter 4 in such a way as to focus on those scientific inquiries where symmetry inferences were used.

To do so I will try to emulate the features identified above that are found in the best examples of historicized epistemologies of concepts — that is, by noting the inferential practices that are facilitated by a given concept of symmetry, by regarding later senses of the symmetry as variants or descendants of earlier ones, and by identifying the mechanisms of that hold the concept stable or drive changes. I will also remain vigilant to known sources of error.

Inferential Practices

To identify the concept of symmetry through inferential practices, we need to analyze the history of research programs. This is because an inferential practice, properly so called, must be evidenced not just in individual inferences but in all the inferences of some specified type that a research community does or could use. Examples of research programs in crystallography are those of Haüy, in the French molecular school, and of Weiss and his associates, in the German dynamist school; examples of research programs in mathematics of the nineteenth century are those of Legendre in solid geometry and of Camille Jordan (1838-1921) in group theory.

To analyze research programs according to the features observed in historical epistemologies of concepts, we would need to set out our account in historical, programmatic, and evolutionary terms. That is, unlike Popper's account, it needs to unfold historically and to treat entire research programs, not merely individual conjectures, as the units of analysis; yet, unlike Kuhn's historical account, it would need to recognize the continuity between successive research programs and actually seek an understanding of the mechanisms underlying those successive changes. Lakatos, who was a highly influential philosopher of science in the latter part of the twentieth century, found a way to steer this middle course between those other once-dominant rival accounts of Popper and Kuhn. His *Methodology of Scientific Research Programmes* (MSRP) provides several of the ideas and distinctions that we need in order to make the important features of a historicized epistemology of symmetry salient.[10] His ideas also facilitate a comparison between developments in science and those in contemporary

[10] I will explain some of Lakatos's more idiosyncratic terms as needed but will bypass certain separable claims that are not relevant to my inquiry (like the rational reconstruction of history).

mathematics — we might have guessed as much by the fact that although Lakatos was known mostly for his work on science, he was initially a philosopher of mathematics known for his work on the methodology set out in his *Proofs and Refutations*, a heuristic of conjectures, proofs, and refutations that is very much like the theories, empirical tests, and anomalous results of science itself.

The MSRP adopts a historical approach. We start, in a Deweyan fashion, with a 'problem situation,' not a definition or an axiom — which is the way a concept like symmetry will be used in material logic. Lakatos names dubs a new way of viewing a problem as a 'problemshift' following which we receive feedback in the form of critique and empirical testing. Unlike the Kuhnian 'paradigm shift,' which is a non-rational move to a new and incommensurable way of viewing the problem, or a Popperian conjecture, which is a psychological process beyond philosophical analysis, a research program developing in an MSPR-like way is one that has comprehensible changes within an identifiable continuity. There are three particularly useful resources on which we can draw when we frame a conceptual history of symmetry in a broadly Lakatosian way.

The first is progressiveness, MSRP's historicized notion of success at the level of the program. Program success is important because it underlies all the types of symmetry warrant we identified previously (§2.3). Using terms similar to those of Lakatos, I recognize a research program as 'progressive,' i.e., successful, insofar as its models can be successfully applied to more cases than the ones used to develop the models the first place; and as 'degenerating' if continued empirical corroboration of the models can be achieved only through positing additional assumptions or parameters *ad hoc*.

Problemshifts, and successions of them, can also be regarded as progressive or degenerating if they lead towards or away from the corresponding research programs.

The second is MSRP's way of treating anomalies, one of its central characteristics. According to Lakatos, in a scientific program there is a 'hard core' of beliefs that define it as being that particular program. Hard core beliefs are defended to the utmost using a 'protective belt' of auxiliary assumptions (including approximations, idealizations, ways of accounting for experimental error, and initial conditions) that can be adjusted or even sacrificed to protect the scientific program from empirical disconfirmation. As long as the research program continues to provide descriptions of new phenomena it will be 'theoretically progressive' and insofar as those descriptions are corroborated it will also be 'empirically progressive.' When it is not, the program becomes a 'degenerating' one. A new problemshift is called for, and if this cycle can be successfully repeated to meet the same criteria the scientific field[11] will be progressive too. Lakatos illustrates this dynamic for the Newtonian Mechanics research program, with its hard core of laws and protective belt of approximations and idealizations, but it is equally applicable to the research programs that gave rise to symmetry concepts, such as those in crystal structure and electric and magnetic fields. MSRP's way of treating anomalies suggests a hypothesis about the conceptual adaptation of symmetry: symmetry adapts in order to reduce anomaly in the scientific research program in which it is embedded, i.e., to

[11] Lakatos uses the term 'programme,' with British spelling, to denote the long-term development of the science that may span many successive research programs, each defined by its own theoretical approach.

maximize inferential success. If a change in symmetry concept can be employed to make a problemshift in the scientific research program that reduces the number of its *ad hoc* assumptions, that conceptual change will continue to be used. We could say, in this sense, that such a conceptual change in symmetry is ‘corroborated’ by the progressiveness of the scientific research program it models.

The third concerns the related idea of heuristic counterexample. Lakatos defends the creative aspect of counterexamples — and this too is what researchers in the physical sciences need if they are to transform their concepts of symmetry in response to earlier failed symmetry inferences and thereby to improve their future inferential success. In the method of *Proofs and Refutations*, Lakatos emphasizes discovery over proof, searching instead for counterexamples to conjectures (which may even be ‘theorems’ if proofs have already been given). When one is found, we may, according to Lakatos, seek to identify a hidden ‘guilty lemma’ in the deductive inference that is falsified by the counterexample, with a view to incorporating it as a presupposition in a revised proof so as to exclude the counterexample. Analogously, in his *Methodology of Scientific Research Programmes*, into which he imported the above ideas on heuristics, Lakatos emphasizes the importance of anomalous experimental results.

Anomalies, as mismatches between observations and expectations, are always important to science because they provide opportunities to locate the cause of the mismatch within our processes of inquiry and thereby to ameliorate those processes. Many mismatches can be fairly explained away by using the ‘protective belt’ (e.g., by fairly attributing them to experimental error or experimental artifact); when that cannot be done in a principled way, we need to modify or even abandon one *or other* of our 'hard core' assumptions. What Lakatos emphasizes is that we should consider the full range of those alternatives, as some may afford us more creative opportunities than others (e.g., by revealing the presence of important assumptions of which we had not previously been aware). When we are faced with a failed symmetry inference, for example, we should be open to the possibility that rather than adjust one of the scientific concepts or mathematical lemmas to remove the anomaly, we should adjust *the concept of symmetry.* 'Shocking' historical counterexamples illustrate this choice.

- Ørsted's demonstration of magnetic deflection, for one, is consistent with symmetry inferences only if we abandon the simple geometric concept of the physical symmetry of physical forces that had been implicitly modeled on that of the little arrows we traditionally use to represent forces (Altmann 1-40).
- The discovery of fivefold symmetry in certain crystal-like substances was a counterexample to the Crystallographic Restriction Theorem. Yet this 'anomaly' was not a body blow to crystallography; it was a creative opportunity. It had exposed the facile assumption, seldom consciously pondered before, that all space-filling assemblages of parts had periodic lattice structures. Once the mathematical possibility of aperiodic space-filling patterns was recognized, the field of quasicrystals was born.
- Archimedes succeeded in his work because the physical symmetry of gravitational forces is analogous to the geometric symmetry of arrows used to represent them.

I intend to analyze inferential practices that were historically situated. One clear risk in doing this is inadvertent anachronism. Since the case study is on nineteenth-century crystallography, I have identified a number of interpretative issues concerning the literature of that field in that period intended in order to minimize the risk of making anachronistic judgments (see §3.5 below). I have also specifically addressed the risk of inadvertently using rational reconstructions instead of historical accounts (§3.5).

Continuity and Replacement

To say that symmetry itself has a history, we need to specify the features shared by concepts of symmetry that succeed one another. Although clearer indications of these shared features should emerge from case studies, common usage suggests that a symmetry is a principled way of deeming two or more non-identical parts, states, or points of view to be equivalent for some stated purpose (Chapter 1). Expressed conversely, what seems to be common to concepts we regard as types of symmetry is the identification of aspects of the problem situation that are *ir*relevant for the purpose we have. The variant or descendant concepts differ in how that is done and for what purpose. Where this or any other concept does develop over time, as opposed to simply being terminated or replaced, it is important to highlight the continuity as a guide to searching for the mechanisms that maintain conceptual constancy or drive conceptual change.

The opposite error is failing to acknowledge differences important enough to affect the validity of the inference. One source of such errors, identified by Mark Wilson in *Wandering Significance*, is 'property dragging.' In the case of symmetry, property dragging would be any tendency to misattribute to one variant of symmetry the properties of another one. I have identified some examples of this (see §3.5). We should avoid making such errors ourselves, but if the researchers being studied made them we should note that as those errors could inform us about the historical processes of conceptual change.

Mechanisms that Maintain Constancy and Mechanisms that Drive Change

To explain the stability of or change in the concept of symmetry over time, we need to posit particular mechanisms for which evidence (for or against) may be found in the historical record.

To frame the search for the mechanisms underlying the projectable warrant, imagine a scientific research program (in crystallography, say) where a particular concept of symmetry facilitates inferences (about, say, shape or other crystal properties). The researchers try to maintain the progressiveness of their existing research program, i.e., they try to maximize the number of corroborated symmetry inferences and to avoid unresolved anomalies. In the short term, to defend the use of a particular concept of symmetry (said to be part of the Lakatosian 'hard core' of their scientific research program) they explain away any apparent anomalies by the operation of other factors, like experimental error, imperfections in crystal specimens (said, for these reasons, to be part of the Lakatosian 'protective belt'). In the longer term, they may use a number of adaptive mechanisms in an effort to preserve the program. As Hacking expresses it, in terms of theories:

> Our preserved theories and the world fit together so snugly less because we have found out how the world is than because we have tailored each to the other. ("Self-Vindication" 31)

Hacking then lists many practices that comprise what he terms 'self-vindication' of the laboratory sciences, ways in which we achieve a "snug" fit by structuring the empirical arena in a way that makes corroboration possible. In the example of crystallography, one stratagem has been to structure the field so that it applies only to crystals grown in the laboratory under standardized and controlled conditions that eliminate the pesky crystal asymmetries found in the wild and to develop experimental protocols for establishing symmetries. In any case, we should not prejudge any of these protective-belt or self-vindicating moves but merely remain alert to their possibility and allow the historical records to speak for themselves.

To frame the search for mechanisms underlying the evolvable warrant, imagine that the research program — perhaps now challenged by the increased precision of measurements or by new phenomena — can no longer be defended by protective-belt or self-vindicating moves. It has, let us say, slipped into being a degenerating program because it is sustained only by the continuous infusion of *ad hoc* assumptions and parameters. The researchers, perhaps from a different school, now try to replace the program with a progressive one by adjusting what was formerly in the hard core. This adjustment could of course be made to any of the elements of the hard core of the scientific program. But if the adjustment falls on the symmetry concept itself we may want to look for the mechanism[12] that makes that *repeated* change of *that* concept

[12] While it seems unlikely that the historical record in crystallography is rich enough to illuminate this particular issue, that of high-energy physics suggests that the self-vindicating strategy is a commitment to keep explaining recalcitrant symmetries at one energy level by invoking evermore inclusive symmetries at higher levels.

possible. That is, a mechanism to explain why it is that symmetry can be relied on to adapt continually. Why not just replace it with something completely different? (It is beyond the scope of the current project to do this because a larger sample of research programs would be needed to establish the mechanisms involved.)

Finally, to frame the search for a mechanism for the transferable warrant, imagine that the symmetry inferences from a successful research program in one domain (crystallography, say) were used in another (electromagnetism, say). The mechanism for this to be possible would seem to be completely decoupling the symmetry inferences from the material context of the source domain and re-attaching them by interpretation specific to the target domain. That is, in effect, the symmetry inferences would no longer be material at all but purely syntactic, mathematical in fact. (It is beyond the scope of the current project to do this because the transfers occurred in a later time period, after Pierre Curie instigated this transfers to physics.)

Specifically, I narrate the emergence of the scientific concept of symmetry in the following way. The starting point is a problem situation of the science, which is taken as the driver of a dialectical process of conjecture, counterexample, and response in the science as well as in ways to model it. Then a problemshift, a conjectured way to address the problems of the science, is described. Since we are exploring the role of symmetry, I will be selecting cases for which this problemshift is made possible by or described in terms of a symmetry concept used to model it, whether that concept is inherited from an earlier phase of that science or introduced as a metaphor from outside. Symmetry is used in the hope that it makes the science ‘progressive’ in Lakatos’s sense, i.e., that it has excess inferential capacity, the ability to make successful inferences beyond the ones it was specifically tailored to make. Counterexamples to those inferences could require adjustments to the science or the way it is modeled, such as to the symmetry concept employed and consequently to the mathematics used to describe its application to the physical situation.

3.5 Further Details and Potential Objections

Avoiding Anachronism

There are a number of pitfalls in reading the scientific literature on crystallography in the nineteenth century. We need to be aware that some terms — like ‘atoms,’ ‘molecules,’ and even ‘crystal’ — did not have the same connotations they have today and that symmetry inferences were made in the context of scientific models that have been superseded.

The Problem Situation

The most obvious anachronism, but the one that is easiest to correct, is projecting back our problem situation. Researchers in the nineteenth century did not have access to current techniques like X-ray diffraction, newer concepts like color symmetry to help enumerate the subgroups of crystallographic groups, or more recent notation such as the *International tables of Crystalline Structure*, to help sort out the profusion of systems that have evolved. The overwhelming success of X-ray diffraction techniques in the twentieth century has shifted the focus of crystallography away from the earlier issues of describing and explaining the external form of crystals to describing the classifying the internal structures that account for those external forms. So, even when not focused on the subfield of X-ray crystallography itself, introductory surveys today typically begin with the internal structure of a definition of a crystal in terms of its periodic structure. (See, for example, Borchardt-Ott, Sands, and Szwacki and Szwacka.)

In the nineteenth century, however, the problem situation was to account for macroscopic phenomena observable in the laboratory, originally crystal form but also elastic deformation, electrical and thermal conduction, and various optical phenomena. Particular internal structures, together with their symmetries, were the hypotheses. Therefore, presenting the subject in reverse chronological order, although no doubt pedagogically effective, tends to obscure the actual inferential process. As F. C. Phillips laments in Preface to the First Edition of his text of 1946:

> The fact that the main centre of interest in crystallographic studies has been changed by the discovery … of the diffraction of X-rays by crystals is indisputable. As a consequence, the belief is now widely held that the external morphology is no longer of interest or importance, and we are urged to adopt a 'new view-point' and to begin the study of crystallography in terms of the structural pattern of crystals. … It is not the least serious drawback of teaching from [this] 'new view-point' … that the student is asked to accept at the outset so much that he cannot immediately grasp for himself. He cannot see and handle the atomic structure, and check for himself the regular arrangement, in the same direct way in which he can handle the crystals themselves and check the regularity of the angular relationships of the faces by direct goniometrical

> measurements until the existence of an orderly structure in the crystalline state becomes something much more real to him than a plausible explanation of certain diffraction effects (Phillips, Fourth Edition, vii).

A partial solution to this potential source of error is to make use of near-contemporary sources. Wadsworth's 1909 text on crystallography was based on his 1873 lectures and his problem situation was the mineralogical one of determining, for the purpose of further inquiry or prospecting, the real external form of a crystal, given that the sample that might be rough or broken. He is also sympathetic to the Phillips's sentiment concerning the desirability of laboratory culture. It's likely that the presence or absence of laboratory experience affects the appreciation if not the meaning of geometric concepts such as form, structure, and symmetry. Walker's 1919 textbook likewise highlights hands-on methods and the problem of identifying crystal form.

Atomism

Another anachronism concerns the presupposition of atomism. The atomic theory of matter is foundational in crystallography in the twentieth century, especially following the game-changing invention of X-ray diffraction techniques in 1912. It had also become increasingly mainstream in the nineteenth century in the wake of chemical discoveries, and so we need not doubt that many crystallographers in the nineteenth century held such a view. Atomism is assumed background in modern texts; older texts like those of Wadsworth and of Walker, focusing almost entirely on external form, do not invoke atomism; and some works use 'atom' to refer to an indivisible or unanalyzed unit and 'molecule' to refer to a geometric unit of analysis rather than apply these terms as we do today.

The most important danger is that taking atomism to be the default description may obscure the nature of the inferences crystallographers were required to make at the time they made them — in particular, whether their inferences were regarded as *a priori* or essentially empirical. Some inferences may, for example, be valid for purely geometric reasons and do not require us to suppose that it is actual atoms in the modern sense determine crystal structure. It is common to regard crystals geometrically as periodic arrays of unit cells, rhomboids defined by characteristic lengths in each of three directions that do not lie in the same plane. It is also common now to regard atoms as marking out those unit cells. Both the unit cells and atoms are constitutive of the crystal and 'indivisible' in their own ways, geometric and physical. But neither the cells nor the eight points in three-dimensional space that mark the unit cells out are equivalent to physical atoms: for example, unit cells are space-filling while atoms are not; the points marking out the cells are infinitesimal while atoms are extended; and unit cells are conventional — alternative constructions being possible — while atoms are not. We shouldn't just assume that a symmetry inference, even one that is discovered empirically, is actually empirical, let alone based on the atomic nature of matter.

Because crystallography developed first to account for external morphology, I generally interpret inferences geometrically as far as this can be done and include atomism only when the context requires it.

Domain

A third issue, which is more general than that of atomism, concerns the too-quick assumption that a problem-situation resides in the domain of physics. Because the inherited notion of symmetry is a geometric one, we need to determine whether the symmetries and forms about which we are reasoning are themselves geometric or, as is sometimes supposed, 'physical' and 'out there.' Because 'crystal' commonly connotes a body bounded by plane faces and not just a form, it is important to distinguish between forms that are impossible (because, say, a certain combination of defining symmetries cannot co-exist for mathematical reasons) and forms that are merely absent in nature (perhaps because the laws of nature do not favor them). The casual use of 'crystal forms' to denote forms of interest may obscure this distinction.

External Form and Internal Structure

The last issue is the conflation of external forms with the internal structures that purportedly give rise to them. This is occasioned by the shift in the focus of crystallography from crystals, finite bodies bounded by plane surface, to crystal structure, a periodic array of atoms extending (ideally) infinitely in all directions. But with 'crystal' now more of an adjective than a noun, it is not always clear when it refers to external form and when to internal structure. Until the twentieth century, crystallographers classified crystals by the symmetries of their external form, while accounts of such crystal form are now more usually given in terms of internal structure, unit cells defined by a lattice of points. Confusingly, the same technical terms can sometimes refer to both a crystal form and to a lattice system.

Using Rational Reconstruction Appropriately

A rational reconstruction, as I will use the term, is a re-description of an extant science in terms of *new* concepts in order to demonstrate or highlight the logical connections among the concepts used in that science. Such re-descriptions are, therefore, avowedly anachronistic rather than historical. Rational reconstructions are generally motivated by the drive for unity, clear exposition, or the effective pedagogy rather than any historiographical concerns. Although presented as a sequence — describing certain facts or laws as ‘following’ from a small number of ‘initial’ assumptions — this form of presentation is just a manner of speaking. The sequence presented is logical rather than chronological and, if construed temporally, it is counterfactual rather than historical. As Mark Steiner puts it, in introducing his own reconstruction of quantum mechanics:

> There is nothing historical … about the following ‘derivation’ of quantum mechanics … On the contrary, I reverse the historical order to show that, starting with little more than the ‘Maximality Principle,’ quantum mechanics could have been discovered by studying the formalism itself, rather than studying nature (177).

Although a rational reconstruction, in the sense described above, is not a historical account of an earlier time, it is a historical fact about its time when the reconstructing is done. The arrival of a rational reconstruction may signpost the recent origin of the concept that makes such a reconstruction possible or desirable. Consider the following examples. After the algebraic concept of symmetry was developed to solve certain problems in the theory of equations, it was used to reconstruct and unify a plethora of new geometrics that had sprung up in the nineteenth century. The reconstruction does not inform us when or how those geometries arose but it may help date the algebraic concept used. After the symmetry concept had migrated from crystallography to physics, classical physics could then be reconstructed in the form of the Theory of Relativity. After Emma Noether had proved her famous theorems linking physical symmetries to specific conserved quantities, new ways of deriving and presenting the fundamental laws of physics became possible.

The following three uses of symmetry, one in mathematics and two in physics, illustrate the variety of purposes for which it is appropriate to do a rational reconstruction. History is not one of these appropriate purposes.

Mathematics

Symmetry concepts, whose mathematical relationships were formalized in what became known as Group Theory, stimulated and formed the basis of a rational reconstruction of the field of geometry itself. Symmetry had once been regarded as primarily a geometrical concept, but in Group Theory had become a more general and more powerful concept, expressed algebraically. Felix Klein (1849-1925), when he became professor at Erlangen University, Bavaria, in 1872, initiated a reconstruction of geometry, bringing unity to the diversity of new geometries that had proliferated in the nineteenth century by using the concept of a group. This reconstructive effort, which became known as the *Erlanger Programm*, re-described geometries as the investigation of those properties of geometric figures that remain invariant under a given group of transformations, i.e., their symmetries, in the modern sense of the word. Any classification of groups thus becomes a way to classify geometries. One simple example is Euclidean Geometry, which has an unstated axiom that areas and lengths remain invariant under a group of transformations in the plane, namely the 'rigid' transformations of translation and rotation.

Physics (Pedagogy)

Jakob Schwichtenberg wrote *Physics from Symmetry*, a rational reconstruction of standard physics, for pedagogical reasons, not to discover any new physics. He re-derives the fundamental equations and theories from a common origin in symmetry, thereby reducing their number and making them easier to learn and remember. His approach, like that of the others, is explicitly non-historical:

> Many things that may seem arbitrary or a little wild when learnt for the first time using the usual historical approach, can be seen as having been inevitable and straightforward when studied from the symmetry point of view (X).

In fact, as it sometimes turns out in rational reconstructions, his book *starts* at what would actually be the *end* of a historical narrative:

> Before we even talk about classical mechanics or non-relativistic quantum mechanics, we will use … exact symmetries of nature to derive the fundamental equations of quantum field theory (IX).

Physics (Unification)

Einstein's relativity revolution was the result of a rational reconstruction of classical physics using symmetries implicit in the theories of electromagnetism and mechanics. That led Einstein to introduce, in 1905, subtle variations of the concepts of space and time to complete a long process of reconstruction that had been started by others, effectively shifting the semantics while leaving the syntax (the broad framework) in place.[13]

It is unfortunate that 'rational reconstruction' has sometimes been offered (notoriously, in case of Lakatos) as a type of history. Whatever terms we use, the important processes I describe and illustrate above should not be conflated with any history of symmetry.

Guarding against Property Dragging

If we view the conceptual trajectory of symmetry not as a random walk through history but as the natural record of adaptations to changing inferential needs, we should be able to identify when those adaptations first successfully emerged from earlier conceptions of symmetry.

Aesthetic Symmetry

The inferential force of aesthetic symmetry is the hardest to defend because that symmetry is subjective. Even if one were to give 'an accounting for taste,' that account is likely to be contingent on our preferences as members of a particular species. Notwithstanding that, properties of aesthetic symmetry are sometimes dragged inadvertently into inferences that are supposedly based on other concepts of symmetry. This shocks us because our expectations of beauty are disabused. For example, earlier 'proofs' of the Four-Color Theorem (the theorem that states, roughly, that one needs no more than four colors to fill in a map so that no two zones will have the same color) were

[13] One recent description of this process can be found in Renn's "The Relativity Revolution from the Perspective of Historical Epistemology."

extremely elegant. Unfortunately, they were demonstrably fallacious. Sadly, for those hoping for beauty, the currently accepted proof is hundreds of pages long, relies substantially on computer-assisted enumeration and checking of possible topological configurations, and is thus (for many people) decidedly ugly. Likewise, many physical theories have been regarded as too beautiful not to be true. In our day, some physicists believe that String Theory and Supersymmetry are in this category, even though the only appropriate criteria are those for empirical corroboration.

The most telling ugliness for our project is at the very heart of algebraic symmetry: the crowning intellectual achievement of Group Theory. This is known formally as the Classification of Finite Simple Groups; less formally as the Classification Theorem; and pejoratively as the Enormous Theorem. Perhaps envisioned initially to be the elegant counterpart to the list of prime numbers in number theory or to the periodic table of the elements in chemistry, the classification assigns each of the finite simple groups, as it were the 'building blocks' of symmetry, to one of four classes. But this theorem and the resulting classification are very ugly in several ways. First, the 800-page proof, a collaborative effort of hundreds of mathematicians over almost 50 years, cannot be absorbed by any single individual in a single sitting and does not have the elegance of a simple proof that generates an 'aha' moment. Second, the fourth class is a 27-member class of 'sporadic groups,' groups that do not fit the systematic pattern of any of the others. Third, the largest of those sporadic groups, the aptly-named Monster Group, has about $8 \text{ x } 10^{53}$ elements and involves the manipulation of a symmetrical mathematical object in a space of 196,883 dimensions — outstripping not only our powers of aesthetic appreciation but also any human intuitions rooted in geometric symmetry. Finally, although one might take aesthetic consolation in the fact that the Monster Group at least contains (in the mathematically precise sense of 'subquotients') 20 of the other sporadic groups, we still have to lament that 6 will remain forever and provably at large. They are known tellingly as 'pariah groups.'

Geometric Symmetry

In the Renaissance, strict bilateral symmetry (mirror-image symmetry) became the aesthetic norm in architecture. It was, we might say, a case of dragging the properties of a geometric conception of symmetry to the aesthetic one. That meant that when inferences were made according to a symmetry that was putatively aesthetic, they could actually be made quite straightforwardly according to a symmetry that was actually geometric. The problem came later. Those who restore ancient ruins often feel the urge to reconstruct a missing piece (a frieze, say) and to do so they need to infer its design from the aesthetic symmetry that would have motivated the original builders. How were the sizes of different elements related? But by assuming, as has all too often been the case, that the design would have been the mirror-image of the piece in a corresponding part of the building, they are guilty of anachronistically assuming that aesthetic judgments of ancient builders were strictly geometric. They were not.

In rational mechanics, to take another example, one makes inferences on the basis of the geometrical icons used to represent gravitational and other forces. The downward-pointing arrows on the drawing of the right arm of a balance are the mirror images of those on the left for points equally distant from the pivot that are suspending equal masses. It is ‘obvious’ to us, as it would have been obvious to Archimedes, on the basis of the geometrical symmetry of those arrows that the balance would remain in equilibrium — there being ‘no more’ reason for the right arm to move down than the left. But one of the properties of geometrical symmetry has been dragged to physical symmetry: apriority. Because empirical corroboration over many centuries has been so extensive, it is still tempting to think of the balance law (and other results of Archimedes’ rational mechanics) as *a priori* and necessarily true. Nevertheless, equilibrium of the balance is actually an empirical result from which we infer that gravitational force is (what is now known as) a polar vector, i.e., that it acts in many respects the way geometrical arrows do. But the same balance apparatus used to balance forces that transform according to different symmetries (for example, torsional forces that one can create by twisting cylinders of suitable material) yields different, non-equilibrium results.

That there is a distinction between physical and geometrical symmetry is obviously very important, the lesson being that we should not impute to physical systems the geometric symmetries of the particular diagrams we happen to use until we have empirical confirmation that the diagrammatic representation of the physical systems is appropriate. An important moment in the conceptual career of symmetry occurred around 1820 when Ørsted performed his famous demonstrations that the deflection of a magnetic compass needle due to an electric current nearby ‘violated’ geometric intuitions based on the symmetry of the experimental setup. We no longer view this as a metaphysical catastrophe that contradicts some synthetic *a priori* proposition, but as a crucial experiment from which we can infer the physical symmetry of magnetic fields.

Persistence in this property dragging caused Ørsted to spend eight years fruitlessly trying to generate the experimental results he wrongly expected.

Algebraic Symmetry

Algebraic symmetries (those permutations of viewpoint that leave some system property invariant) are more abstract and less familiar. That may make them less prone to having their properties dragged unwittingly into other conceptual contexts. Nevertheless, and like geometric symmetries, they are mathematical and may for the same reason give rise to the illusion of apriority when their mathematically demonstrable properties are dragged to physical systems.

Ian Hacking draws attention to the way the algebraic symmetries need to be matched empirically to physical symmetries through a simple illustration from the early days of probability theory.

> In a brief memorandum, [Galileo] relates that someone has been puzzled by a seeming contradiction between two facts. With three dice "9 and 12 can be made up in as many ways as 10 and 11." Each, that is, can be decomposed into 6 partitions. However "it is known from long observation that dice players consider 10 and 11 to be more advantageous than 9 and 12." Galileo's solution is immediate. There is a "very simple explanation, namely that some numbers are more easily and frequently made than others, which depends on their being able to made up with more variety of numbers." In particular the 6 partitions of 9 and 12 break down into 25 permutations, while the 6 partitions of 10 and 11 decompose

into 27 permutations. If permutations are equally probable, then 11 is more advantageous than 12 in the ratio 27:25 (*Emergence* 52).

In Hacking's example, the algebraic symmetries are the various outcomes that are invariant despite the rearrangement of the individual faces. But which is the relevant symmetry: that the outcome '11' (say) is invariant under

Either 6 partitions (the ways three dice throws can add to 11 whatever order the order in which they are thrown) , viz.

641, 632, 551, 542, 533, 443

Or 27 permutations (the ways three dice can add to 11 when we regard the sequence of throws as distinct), viz.

641, 614, 461, 416, 164, 146

632, 623, 362, 326, 263, 236

551, 515, 155

542, 524, 452, 425, 254, 245

542, 524, 452, 425, 254, 245

533, 353, 335

443, 344, 434

Galileo correctly backed permutations, making '11' more probable than '12' in the ration 27:25. Experienced gamblers, who after all have skin in the game, empirically corroborated it. Galileo's method of determining the probabilities of compound outcomes with dice is now so thoroughly confirmed that, as in the case of Archimedes, we forget that it is not *a priori.*

In fact it was by no means obvious that permutations rather than partitions was the right answer. Leibniz, for example, backed partitions for dice, presumably on some *a priori* grounds. And some elementary particles in microphysics, to wit bosons, actually do follow Leibniz's preferred basis of partitions while others, known as fermions, follow a rule that is neither of those discussed above.

4. THE EMPIRICAL CONSTRUCTION OF SYMMETRY

In Chapter 3 I set out the key features for a historical epistemology capable of accounting for the (material) warrants of symmetry inferences. Best practices in comparable historical epistemologies suggest that we need to highlight the way inferential practices are linked to the concepts of symmetry they use; the aspects in which symmetry concepts, successively introduced into empirical studies, are similar to yet different from each other; and the mechanisms driving the changes in the concept of symmetry. To explore the inferential practices in sufficient detail, I identified a number of categories and distinctions (first introduced by Lakatos in the 1970s) that would be suitable for this purpose. These categories and distinctions help one to provide an account that is both historical and conceptual; to take the research program as the unit of analysis, rather than isolated theories and symmetry concepts; and to show how contemporaries judged the scientific successes and failures that drove change in the concept of symmetry and its inferential use.

In this fourth chapter I discuss my choice of nineteenth-century crystallography as a case study (§4.1). The overall argument in this thesis is that the warrants for symmetry arguments are to be found in the processes of inquiry, specifically the co-adaptation of the concept of symmetry and the sciences whose inferential needs it supports; the detailed support for this argument is in the accounts of the symmetry concepts that were introduced in a succession of empirical research programs (§4.2 through §4.4). I then consider a plausible objection to that empirical hypothesis, namely the claim that the concept of symmetry actually arose in mathematics and was only subsequently applied to the empirical realm (§4.5). I conclude with some remarks on the subsequent scientific research programs that treated a variety of physical symmetries. These programs hold the key to understanding why it is that we repeatedly resort to using *symmetry* concepts in responding to empirical challenges (§4.6).

4.1 Case Study Material

The framework of analysis I set out can be applied to any field and time period sufficiently rich in source material. The history of symmetry and the histories of science and mathematics do suggest though that there are three broad epochs that are sufficiently dissimilar to merit separate investigation. The first begins in ancient times, before the advent of science, when ideas on symmetry were driven largely by philosophy and logic. The second begins with the first systematic use of symmetry inference in crystallography in 1801, when the development of the concept of symmetry was driven largely by science. The third can be conventionally dated as starting in 1901, when dramatic discoveries transformed crystallography and physics and the status of symmetry concepts within those fields.

I have chosen to focus on the science of the nineteenth century. This is the formative period for the scientific concept of symmetry; studying it will help clarify what is distinctive about the concept of physical symmetry that subsequently emerged in the latter part of the nineteenth century and the various abstract symmetries that emerged in the twentieth. It will also help focus and motivate any future study of symmetry and related concepts in earlier periods. I turn now to specify the case more precisely in terms of the time period and scientific fields covered.

Time Period

The case study spans the nineteenth century, as this was when the concepts of symmetry used in the physical sciences were developed. Crystallography, the main formative influence, began only in 1780 when Haüy published the first truly scientific work in the field, a mathematical theory to explain the external form of crystals. In 1801 Haüy published the first work making use of symmetry inference. The nineteenth century also saw the development of electricity and magnetism, a field that benefitted greatly from crystallographic symmetry arguments.

Around the turn of the century, discoveries in the sciences created a different environment for the use and further development of symmetry. In 1894 Pierre Curie helped spread the use of symmetry inferences from its native domain of crystallography to the broader domain of physics; in 1905 Albert Einstein made the special status of symmetries in physics apparent; and in 1912 crystallography itself was utterly transformed when the German physicist Max von Laue discovered the diffraction of X-rays by crystals, a discovery that changed the main focus of that field from the external form of crystals to the internal structure of matter. Although mathematical systems to represent three-dimensional spaces and their symmetries had originated in the nineteenth century, it was not until the *twentieth* that Group Theory (the ‘language of symmetry’) and allied branches of abstract algebra really flourished and when mathematics led the further development of the symmetry concept.

Scientific Fields

The case study focuses mostly, but not exclusively, on crystallography, as this field was the crucible for ideas on symmetry for the physical sciences. Curie was right to imply that there had not been any systematic attempt before then to use symmetry arguments independently in other subfields of physics. They had, however, been used to account for various types of physical phenomena insofar as they occurred in crystals and were related to the symmetries of crystal structure. These phenomena included pyroelectricity — the production of electricity through heat; piezoelectricity — the production of electricity through pressure, which Curie himself studied along with his brother; electrical and thermal conductivity; and elasticity.

Sciences other than crystallography and associated fields of classical physics are also relevant to some extent. Mineralogy is sometimes referred to, mainly because crystallography emerged from mineralogy in that period and the boundary between the two was not as clear then as it is now. Chemistry is relevant to the extent that the chemical composition of crystals partly defines their symmetry and because the symmetries of the 'molecules,' as variously conceived at that time, depended on it. Some other fields were indirectly relevant because they influenced the development of concepts; the classification schemes of botany and geology, for example, were used as models for those of crystals. As Bensaude-Vincent and Stengers lament in their *History of Chemistry*, it is often assumed that we can just write a history of each science separately. But we risk overlooking fundamental problems that way. “The historian of science, by accepting the contemporary framework of disciplinary boundaries, tends to take for granted a structure that was pieced together with considerable effort in the past” (3). Fortunately, many of the key players in crystallography combined interests and skills in mathematics and a wide range of sciences. Haüy, for example, had a background not only in mineralogy but also in botany and geology (hence his interest in classification) and Pasteur was a biologist, microbiologist, and chemist. Curie himself was a physicist with considerable mathematical interests. Through his brother Jacques, Curie had access to a laboratory and understanding of chemistry and mineralogy.

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The following three sections constitute the main argument showing that the scientific concept of symmetry has been constructed empirically through its co-adaptation with the sciences whose inferential needs it supports. I do this through a historical epistemology whose broad features were set out in Chapter 3. I begin with an aesthetic notion of symmetry in pre-scientific crystallography (§4.2 below) and then discuss the geometric (§4.3) and algebraic (§4.4) notions in scientific crystallography.

4.2 Aesthetic Symmetry

Crystallography and the scientific concepts of symmetry and form developed together in the nineteenth century. They built on past discoveries and on certain prevailing ideas, some very ancient. The past discoveries included a wealth of descriptive data on crystals that had been studied for thousands of years up till then; it was only in the nineteenth century that crystallography became a science, as it was only then that the reflecting goniometer permitted very precise measurements to be made of the interfacial angles on crystals and only then that mathematical tools were available to facilitate the analysis of quantitative hypotheses about crystal structure. The prevailing ideas were conceptual resources that could be used or adapted for use by the new science — but which could also mislead when applied too loosely. Those of special relevance were two: the concept of symmetry, which up till then had evolved to serve artistic, architectural, and mathematical ends; and the concept of form, which had developed over the centuries from Aristotle's hylomorphism, often in response to pre-scientific inquiries into crystal structure. Both the concept of symmetry and the concept of form continued to develop in the nineteenth century.

The Ancient Problem Situation of Crystallography

The problems posed to the inquiry we now know as crystallography determined its inferential needs and therefore the concepts best suited for those inferences. Although there was no scientific inquiry as we now know it in classical times, there was considerable fascination with crystals, whose symmetries were aesthetically appealing. Although no 'progressive research program' resulted from that fascination, we see the earliest setting of an agenda for crystallographic inquiry, one that persists.

The first type of problem concerns the external form of crystals: how we should describe, value, and explain the presence and variety of crystal forms. In the sixth century BCE, the Pythagorean School, during an "important upswing in mineralogy and all other sciences" (Schuh 14), viewed the cosmos in terms of the five maximally symmetric polyhedra (i.e., the 'Platonic' solids — the cube, tetrahedron, octahedron, icosahedron, and pentagonal dodecahedron). But nothing lasting developed out of that claim; crystals themselves did not become the object of systematic inquiry, remaining merely as objects mentioned in literary and philosophical works.

The second concerns the classification of crystals. Theophrastus (381-287 BCE), Aristotle's successor at the Lyceum, wrote the oldest treatise on minerals in the West, *De Lapidibus*.[14] There he presents a classification of minerals. He divides minerals into the classes of 'earths' from 'stones' and identifies around 50 'species' altogether, including many crystals. What makes this work important for us is neither his specific taxonomy nor his theory relating aesthetic appearance to purification processes of mineral formation but the fact *that he made classification itself a subject for serious inquiry*. What makes his inquiry almost modern is that it is methodically done on the basis of geometric and physical properties, rather than magical ones. In fact, his work was so meticulous that "it is possible to apply modern names to the species [he] described … and to read the Classical theories about [those minerals]" (Schuh 17-18).

The third problem concerns the relationship between crystal properties and crystal structure. Expressed as a general question about the relationship between 'outer appearances' and 'inner reality' this is, in the western tradition, at least as old Parmenides, who flourished around the late sixth century BCE. As a more specific question about appearances and internal structure (the organization of otherwise unanalyzed units), it goes back to Democritus, who flourished shortly thereafter.

[14] Neither Plato (whose Academy was not, in any case, focused on the natural world) nor Aristotle made any significant remarks about crystals.

Shape (external form) is one of the most easily recognized appearances of a crystal, and so its relationship to structure (internal form) would have seemed obvious — especially since both shape and structure are expressible in geometric terms. As Emerton notes, the belief that external form and internal form are related

> is shown by the use of the same word 'form,' like its equivalents *eidos* in Greek and *forma* in Latin, to signify both the outer shape of a thing and also its inner nature or essence. (19)

In fact, even in current literature, it is not always apparent which 'form' is being referred to.

Although the problem of relating external appearance to internal structure is hardly unique to crystallography, there are, as Emerton notes,

> two classes of natural objects that are outstanding on account of their constant and specific outward form, which seems to presuppose as its source an equally constant and specific inward form. These are living creatures and crystals: a human being, an oak tree, or a rock crystal has an instantly recognizable characteristic appearance. (20)

Furthermore, she notes, crystals do not have the myriad complexities of biological objects and so we may guess that they present a clearer way to test theories of that relationship.

This problem is presented most starkly in terms of the observed symmetry of shape. For Johannes Kepler (1571-1630), the author of the first modern work on crystal structure, *The Six-Cornered Snowflake*, the question is "why snowflakes, when they first fall, and before they are entangled into larger clumps, always come down with six corners and with six radii tufted like feathers" (33). This external symmetry cannot be just some random occurrence, Kepler thinks, because that would not explain why "they always fall with six corners and not with five, or seven, as long as they are still scattered and distinct, and before they are driven into a confused mass" (35).

Because crystallographic inquiry was not scientific until the nineteenth century, there were no 'conjectures' that were advanced for methodical testing. We can, however, identify a baseline of conceptual resources available at the time of the birth of scientific crystallography that the earliest scientists used or modified for use. Two important ones were aesthetic symmetry and substantial form.

The Classical Concept of Aesthetic Symmetry

Aesthetic symmetry, as I use the term, is a property of a whole object that results from having proportions that confer goodness, beauty, or elegance to it. As such it is not only a geometric concept but also a normative one at the same time, one that can be used to make inferences about what ought to be the case. The concept (although not the term) is an ancient one — traceable at least as far back as Plato, if not before. We should take note of Plato's pattern of inference because it is representative of one that was sometimes employed in nineteenth-century crystal science — and in the physical sciences more generally, even today.

In his dialogue, the *Timaeus,* Plato uses a concept of aesthetic symmetry to draw certain inferences about the natural world. Although in English translations of *Timaeus* 'symmetry' appears rather infrequently, when it does it is as the translation of συμμετρία, the word from which our word ultimately derives. However, translators commonly render συμμετρία as 'proportion,' rather than as 'symmetry,' because it has both geometric and normative resonances. The geometric sense of συμμετρία is derived from the concept of measurement; the core meaning is found in μέτρον, a concern for measure, or that by which something is measured. But the normative sense is also intended, and so a concept like Plato's συμμετρία would accomplish inferential work in crystallography in two ways. One way would be by privileging what is proportioned over what is not. Plato refers to regular polyhedra and the triangles out of which they can be constructed as beautiful (*Tim*. 53e ff) and suggest that the most beautiful structural theory is the true one; since then, crystallographers have shaped their structural theories with a similar concern for aesthetics. Another way to do inferential work is by yoking together different things on the basis of a supposed common measure. Plato does this for mind and body (*Tim.* 87c-d); by parallel reasoning, a crystallographer could do so for internal structure and external form.

One variant of our first problem is: Why do crystals tend to display so much symmetry? We are tempted to answer this on aesthetic criteria like those used in the *Timaeus* by claiming that proportionality among the physically measurable properties of things is what manifests the order created by the 'craftsperson' of universe — or as crystallographers have since said, established or favored by Nature. As Timaeus recalls, the craftsperson does this by judicious use of proportionality, that is, by maximizing the number of ways every object is related through proportionality, not only to itself but also to everything else (*Tim*. 69b).[15]

A form of inference that was purely geometric developed later. Hon and Goldstein, in their history, describe a 'mathematical path' that leads out of the work of Plato and through that of Euclid, Archimedes, and Kepler (among others) to the concept of geometric symmetry (69-72). They also distinguish an 'aesthetic path' that leads out of Plato through Aristotle and others to a purely artistic concept (93-110). Hon and Goldstein claim that the two concepts of symmetry, tightly bound in Plato, were not clearly distinguished until Roman times, when Vitruvius introduced the term *symmetria*, a transliteration of συμμετρία, for the artistic concept and *commensuratio*, a partial translation of the same word into Latin, reserved more for the geometrical concept (93). Although we claim to use the latter concept in symmetry inferences in the physical sciences today, we need to keep this conceptual ancestry in mind and be alert to the possibility of inadvertent or unsupported 'property dragging' of aesthetic considerations into otherwise warranted geometric inferences.

Kepler himself obviously felt the tension between the two concepts, but after proffering his tentative structural explanations for snowflake symmetry based on geometrical and physical explanations, added:

[15] In this passage and elsewhere, Plato uses cognates of both συμμετρία and ἀναλογία to refer to proportionality and its close synonyms.

> I suspect that these explanations based on material necessity are sufficient, and thus I do not feel the need at this point to philosophize about the perfection, beauty, or nobility of the rhombic figure … (65).

Aesthetic symmetry is still used to make judgments about theories today. Simple theories, for example, are preferred over gratuitously complex ones. Such judgments are problematic only when they masquerade as inferences about the physical world itself, such as when an aesthetic concept of symmetry (balance, elegance, simplicity, etc.) is used to winnow hypotheses that are currently untestable (or, worse, when empirical evidence is contraindicative) on the grounds that it would be 'fitting' that Nature operate in a particular way. Such aesthetic inferences are generally used informally and without explicit acknowledgement of any warrant.

Substantial Form

The substantial form of an object is, loosely speaking, the form that makes it the thing that it is. We understand intuitively the difference between this and its opposite, accidental form, which merely describes the way the object happens to be. Thus a lump of calcium carbonate may be described as large or small, shaped like a brick or broken — these are accidental qualities. But if (in terms of today's understanding) its molecules were arranged in a very specific pattern (*C*) we have a crystal of calcite; arranged in another (*A*), aragonite. These two crystal substances consist of the very same material but have very different physical properties, properties that would not survive a switch in the molecular patterning between *C* and *A*. The *C*-pattern is the substantial form of the material calcium carbonate that makes it calcite. Symmetry may be an aspect of the substantial form of an object (as in the case of calcite) or part of the accidental form of an object (as in the case of a 'crystal' made from cut glass).

The importance of substantial form is especially evident in the third of our crystallography problems. That problemshift was a move away from just describing and classifying crystals by their appearance to accounting for the relationship between appearances (crystal shapes) and 'reality' (crystal structure). If we can regard the substantial form as the internal form, describable as an invariant geometrical arrangement, this relationship will then be a mathematical one from which we can deduce the various external forms compatible with that internal form. With this understanding of the task of crystallography, its development prior to the nineteenth century could then be 'rationally reconstructed' as the quest for the substantial form of crystals that has two aspects to it: "the forms of the molecules of crystals and the way they are arranged together in each crystal. It is this combination that is called structure" (Haüy *Essai* 9, qtd. in Emerton 259).

Emerton writes an inner history of the pre-scientific concept of form, starting with the notion of Aristotle's that united matter and form and moving through the Scholastic elaboration of the notion of substantial form. Although, in the general reaction to Scholasticism, substantial form was heavily attacked, the concept of some sort of internal structure for minerals actually revived in the sixteenth century due to "increasing interest in crystals, coupled with an awareness of the shortcomings of mechanical explanations of crystallization" (36). Emerton argues that there were also other reasons for this revival stemming from the inferential demands of chemical and corpuscularian theories, whose needs for a concept of form not only influenced crystallography but also drew inspiration from it (36). Like the concept of symmetry, the concept of form has developed in tandem with the inquiries it serves, rather than on a segregated philosophical track.

The Modern Problem Situation of Crystallography

We are concerned with the scientific concept of form developing in the nineteenth century, immediately following the time period of Emerton's study. A full description of and accounting for the form of a general object would theoretically be an infinite endeavor and unmanageable. But this is not so for an object with evident symmetry because the symmetry alone may characterize an enormous degree of redundancy in the description and in the account that reduces the problem to a finite and practically manageable one. To cite the most extreme case, a body that is stipulated to be spherically symmetric does not require each of the infinite number of points on its surface to be described and accounted for separately; given this symmetry, describing just one point is sufficient.

Crystals display an important subclass of symmetries, so one could have anticipated that crystallography would become an important field in which to study them. We can now identify those inferential practices in crystallography that used and then modified the prevailing concept of symmetry around 1800. Those inferential needs arose in the course of addressing essentially the same problems that had already exercised the minds of the ancients.

Recall the first problem: how to describe the external form of a crystal. Regardless of the way external form may or may not depend on some substantial inner structure, there are definitely some accidental aspects of crystal appearance — such as size and whether it is imperfect or broken. More interestingly, crystallographers needed to explain the observations that crystals had natural cleavage planes and that their shapes could be altered in lawlike ways by beveling the edges and truncating the corners. Alterations in shape like this are accidental aspects as they do not alter the chemical composition or any of the chemical or physical properties of the crystal specimen. That fact calls for a way of specifying the accidental aspects of form -- such as size, shape, and number of crystal faces—from the essential aspects – those that are invariant in that they do not depend on such accidental aspects.

The second (but related) problem of crystallography concerns crystal classification. Taxonomies are most useful when they uniquely identify the substantial properties. One controversy was whether the invariant features of external form were enough to do this or whether any further properties of the material composition and internal structure (i.e., those involving chemical or geometrical categories) were required.

The third problem concerns the way external form and internal form are related, i.e., how material inferences can be made about one from a knowledge of the other. Many of these inference patterns brought into question the Aristotelian notion of a close bond between matter and form — which, in the context of crystallography, is the association between chemical composition and crystal structure. Some substances composed of the same material may constitute completely different crystals, the way calcium carbonate constitutes both calcite and aragonite, supposedly because they have different internal form — a property known as 'polymorphism.' Conversely, some substances composed of different matter can behave in the same or similar ways, the way zeolites of different chemical composition do, because they have the same internal form — 'isomorphism.' Even more puzzling, some substances that not only comprise the same matter but also possess the same internal form of that matter, may also have different physical properties.[16] And some permissions and restrictions on physical properties and processes can be discerned purely on the grounds of the symmetries in the form of the medium, as happens with pyroelectricity and piezoelectricity in crystals; such inferences being independent of the material composition and even of any particular theory of the phenomenon under study. The mathematization of crystallography in the second half of the nineteenth century made crystal classification and inference a matter of form alone. This is reminiscent of earlier alchemical theories that permitted the in-principle transmutation of elements through detaching form from one desirable element (gold, say) and re-attaching it to a base material (lead, say) — despite the origins of alchemy in Aristotelian thought. It was also not unlike the twentieth-century physics theories that were based on symmetries that were abstract, algebraic forms that are detached, as it were, not only from matter but also from the geometry of three-dimensional space.

[16] An example of this is amyl alcohol. Depending on whether it is prepared by living or non-living processes, solutions of this substance have different optical properties resulting from otherwise identical internal forms being mirror images of each other — a property known as 'chirality.' This was a puzzle that Pasteur helped to solve. See §2.2.

4.3 Geometric Symmetry

The scientific uses of symmetry begin with various concepts of geometric symmetry that were introduced into the crystallography research programme,[17] starting in the late eighteenth century. The general idea was that identical physical conditions of crystal growth would lead to identical outcomes, such as identical geometrical shapes of crystal faces, there being no reason to think otherwise; in uniform conditions, identically shaped faces similarly situated would develop in the same way. This idea obviously had the potential to simplify explanations in crystallography greatly because crystal shapes typically comprise repeated geometric elements.

The Problem Situation in the Mineralogy of the Eighteenth Century

Mineralogy was a branch of geology inquiring into the nature and the theory of minerals, regarded as solid inorganic substances of natural origin. Some minerals are crystals, which are solids bounded by plane faces, typically comprising repeated geometric elements. By the eighteenth century, crystals had become the subject of a subfield of mineralogy.

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[17] Lakatos uses ‘programme’ to refer to a series of scientific activities extending over the long term, without implying that the principal actors see their activities as constitutive of a single endeavor. This is more or less what we mean by a ‘field of inquiry,’ such as crystallography as a whole. I follow the common practice of reserving ‘program’ for activities grouped according to a particular theoretical approach (such as Romé de l’Isle’s and Haüy’s distinctive approaches to crystallography) and reserving the British spelling to mark the broader, Lakatosian sense.

Crystallography then began moving away from mineralogy in two ways: it was specializing in questions such as crystal structure and classification and it was expanding to cover not only natural crystals but also ones grown artificially in controlled conditions.[18] Crystallography in the eighteenth century had been concerned with the classification of crystals by their external geometric form, specifically by their symmetries (understood as regularities). Crystals were regarded as solid bodies bounded by plane faces (i.e., they were polyhedra), and their geometric regularities were determined by measuring the angles between adjacent faces. (Quick identification of minerals by the symmetries they displayed by their crystals would be very useful to mineralogists in the field, where they might not be able to do a chemical assay.) One of the problems dealt with at that time was the first on the ancients' list: that of describing and accounting for the vast variety of crystal forms, especially the variety of forms sometimes associated with what seem to be the very same mineral.

Romé de l'Isle's Research Program

Romé de l'Isle took up the task of classifying crystal forms according to the hypothesis that underlying a multitude of accidental forms ('secondary forms' or 'appearances') there was a small number of substantial forms ('primary forms,' often called 'primitive forms') out of which they were assembled. He noted, for example, that if the crystal itself took the primitive form (a cube, say) it could be systematically

[18] Controlling the growth of crystal specimens, Dewey would say, is a way of preparing the data for material inference. Hacking would cite this as one of the self-vindicating actions of the laboratory science that crystallography had become.

truncated at its weak spots (on its corners or along its edges) to produce a plethora of new forms that, he supposed, were merely secondary to the primitive form the crystal had originally. He hoped to build a classification scheme on well-defined theoretical principles that was based on the invariant features and that ignored the accidental features. This could be used to predict the existence of new crystal forms, i.e., ones that were deemed theoretically possible on that basis even though they had not yet been observed in natural crystals (Burke 74-76).

Romé de l'Isle had a research program with a clear method of proceeding. In his program, the positive heuristic of crystallography was: Describe all the primitive forms and the secondary forms that are related to them. In this way, Romé de l'Isle clearly showed that crystallographic classification was a serious endeavor based on theoretical principles rather than superficial likenesses. He had come from a background in Natural History and was an admirer of the Linnaean system of classification; what may have struck him was the Linnaean use of characteristic features, i.e., the constant and invariable features that allow one to classify a species (Hon, *From* Summetria 56). He was also no doubt aware of the relevant differences between crystal species and biological species — in particular, the fact that the truly invariant features of a crystal are not visible in their external form (which can be highly variable, unlike the case with biological species). Crystal features are geometric, rather than functional as they are in biology, and Romé de l'Isle realized that as such they could be determined quantitatively with great precision using the recently invented contact goniometer. He demonstrated in great detail how a primitive form of a crystal shape could be transformed in a lawlike way to a number of secondary forms through beveling and truncation and showed that the characteristic features of a crystalline substance did not include its appearance (a mere secondary form) but did include its primitive form and sometimes other physical properties as well. As a result of his extensive studies, Romé de l'Isle proposed a classification scheme comprising six primitive forms and showed that known crystalline substances could be included in one or other of these classes.

Romé de l'Isle's Use of Geometric Symmetry

Romé de l'Isle used a geometric concept of symmetry to help with this problem of classification. For him, the characteristic (i.e., constant and invariable) features of a given crystalline substance include its primitive form (which had to be identified from a table of possible forms) and its interfacial angles (which had to be measured accurately). Symmetry for him meant that

> every time that the same combination of the same elementary principles comes to operate in exactly similar circumstances and proportions, we see that there result from it bodies of the same form, the same density, the same hardness, the same flavor, etc.

and that, conversely,

> lacking the conjunction of all these circumstances, crystallization often remains indistinct, imperfect. (Romé de l'Isle qtd. and trans. in Hon, *From* Summetria 189).

That is to say, equivalent physical conditions will lead to, among other things, equivalent geometric features.

The proviso, 'equivalent physical conditions,' requires that the growth and selection laboratory samples need to be controlled in order to minimize any 'accidental' features. That in turn meant Romé de l'Isle's program had at least one defensive maneuver in the 'protective belt': anomalous forms could develop if those physical conditions were not uniform or constant.

Romé de l'Isle's Degenerating Program

Ultimately, Romé de l'Isle's program became a degenerating one.[19] The postulated primitive forms were arbitrary, and so were the theoretical truncations and bevelings that were used to claim that an observed crystal shape was a secondary form relative to a primitive one. In 1803, one near-contemporary reviewer acknowledged that the program was only initially progressive but that it had become *ad hoc*:

> Though often successful in explaining the origin of the most complex secondary forms, by means of imaginary truncations and bevellings of a simple solid, the immense industry and great sagacity of this last inquirer [Romé de l'Isle] were frequently baffled, and he was reluctantly obliged to suppose that some minerals possessed more than one original form, from

[19] As the analyst, I use Lakatosian terms as common descriptors for a variety of research programs. Note, however, that I do not use those categories and distinctions as the basis for any historical claims, i.e., to rationally reconstruct the motivations or specific actions of the historical agents themselves. Because claims about symmetry and about program 'degeneration' are particularly important for my argument, I cite the contemporary or near-contemporary historiographical records that provide direct support.

> which their modifications were deduced. However necessary such a conclusion might appear, it was evidently inadmissible, without supposing a deviation from that uniformity which is invariably found in the works of nature; and even if the system of Romé de l'Isle had been rescued from this mortifying concession, it would still have been wholly unfit for the determination of minerals by their crystals, as few solids would have been esteemed the common origin of numerous substances most efficiently distinct. ("Review of M. Haüy's *Traité de Mineralogie*" 45)

This program degeneration was clearly a factor in choosing between rival programs since, just a year later, when he was reviewing the relative merits of Romé de l'Isle's program and another one, Abbé Buée expressed his misgivings about arbitrariness of the former this way:

> [B]y a series of arbitrary truncations we may pass insensibly from any given form to any other. Grounded on this principle, and seconded by Mr. de l'Isle's ingenuity, any form may become primitive, and any other deduced from it. Now as the combinations are infinite … nothing is proved. (Buée 32)

In other words, the approach was flexible enough to produce any given shape from any other (Burke 77). Furthermore, Romé de l'Isle had no explanatory model and regarded the mechanism of crystal formation as deeply mysterious. It is against that background of failure that we need to view the developments in crystallography that followed.

The Problem Situation in Crystallography circa 1800

The French molecular theory of crystal structure held that there were not just primitive *forms* that described crystals but there were also primitive *particles* that constituted crystals, imperceptibly small secondary particles that were usually taken to be polyhedra. These secondary particles were postulated to be identical in shape and composition to each other. They were believed to bind together to form the aggregates we recognize as crystals; layers of them would be superimposed on other layers in ways that determined crystal shape. The German ‘polar theory,’ by contrast, emphasized forces that radiated from various points in the crystal. Haüy subscribed to the French school and so his theory was built on a geometric conception of these secondary particles, unit cells that fill the space of the crystal. He used it to take up and transform all three of the traditional problems of crystallography.

The first problem, that of describing and accounting for crystal shapes, became for Haüy the task of reducing already known empirical laws about crystal appearances, such as the Law of Constancy of Interfacial Angles, to more basic ones and to account for otherwise brute facts, like the quantified relationships among the various aspects of a crystal. For this task he needed an explanatory model of crystal structure.

The second problem, that of classifying crystals, became the task of systematically reducing the plethora of observed forms to a few elemental ones in a theoretically principled (i.e., non-*ad hoc*) way. To do this he needed to overcome the issues that dogged Romé de l’Isle’s program, which (as we saw above) was generally regarded as arbitrary and qualitative. Haüy's program was explicitly contrasted with Romé de l'Isle's in his own day:

> Before we can determine, whether these [Haüy's] extraordinary innovations are entitled to our unqualified approbation, it is necessary to inquire, whether they were actually called for by the errors of the preceding systems [Romé de l'Isle's], and whether they furnish proper remedies for acknowledged defects. ("Review of M. Haüy's *Traité de Mineralogie*" 43-44)

It was quite clear that grounds for preferring one over the other were the degree of arbitrariness, and that Haüy's is clearly favored:

> The same accuracy of research that has enlarged the number of components, has diminished the estimated number of compounded bodies, by proving the frivolity of many superficial distinctions which had been regarded as specific, and by establishing precise criteria of essential differences. (*Ibid*. 43)

The third problem, that of relating crystal properties to crystal structure, was bound up with the solution of the other problems: the task of relating crystal shape to molecular structure, using a model of Haüy's devising. What makes Haüy's work important for our study is that the solutions he proposed for these tasks eventually required him to use concepts of symmetry in the material context of crystals in a way that comported well with French molecular ideas.

Problemshifts: Internal Structure and Repeated Cleavage

Initially, Haüy shifted the problems of crystallography both theoretically and experimentally; subsequently, in his mature work, he then had to introduce and employ a modified concept of symmetry in an attempt to keep his research program progressive.

Theoretically, whereas Romé de l'Isle had focused only on the external form of the crystal and tried to account for the myriad guises in which the 'substantially' same crystal might appear when 'accidentally' bevelled or truncated, Haüy focused on the *relationship* between the external form and its (hypothetical) internal structure. Specifically, Haüy pondered permissible ways in which the primary forms of the constituent parts could be configured to yield the shapes of the whole. Specific hypotheses about internal structure would be testable: they would have to account for known external forms, predict other external forms that were possible even if not yet observed, and rule out yet others as impossible.

Experimentally, whereas Romé de l'Isle and others had noted that crystals could be cleaved along weak planes to change the external form, Haüy experimented with *repeated* cleavage, conjecturing that this would eventually reveal the truly primary form of the constituent parts (asymptotically, as it were). Haüy's initial (but probably apocryphal) Eureka moment occurred when he is said

> to have dropped and broken a group of calcite that had crystallized in the shape of hexagonal prisms. As he stooped to pick up the debris, he noticed the fragments were rhombohedra corresponding in every detail to the shape of the Iceland crystal [known now as Iceland spar, a transparent

> variety of calcite]. Immediately the idea came to him that such rhombohedra must be the nuclei of all calcite crystals. (Burke 83)

This procedure could not explain why crystals had the primitive forms they did, but it was still a great improvement. A contemporary reviewer praised him for avoiding the arbitrary choices his predecessor would have to make:

> The Abbé Haüy does not undertake to prove generally, that among the different crystalline forms of the same substance, one of them is the primitive; but he produces that primitive form from each crystal, which is always similar in similar substances. (Buée 33)

Haüy shifted the problem of codifying the regularities observed in crystal form from empirical laws to scientific explanations based on an internal structure that had been hypothesized on the basis of experimental data pertaining to the substance in question. These explanations would have, in the Lakatosian lexicon, an 'excess empirical content,' meaning that they unified existing laws and predicted observations not already used in the development or calibration of the model. Before describing Haüy's novel use of symmetry concepts though, it will be necessary to first set out his proposed explanatory model and his proposed classification scheme, because it is problems in his initial proposals that led him to introduce symmetry and which explain the material context of inferences that he proposed to make on the basis of symmetry.

Haüy's Crystal Model

Haüy used his model to explain the particular variety of observed crystal shapes. Haüy modeled crystals as structures built from blocks deposited in successive layers on a nucleus in a regular pattern. So Haüy needed to posit two things: a shape for each building block (including its plane and interfacial angles) and a pattern of layering. The mere existence of primitive forms and layering was sufficient for his inferences and he did not offer any explanation for either.[20]

The building blocks, Haüy initially thought, were just the primitive forms. Using the primitive form had worked well for calcite and its other crystal varieties. But Haüy was forced to make two further theoretical moves. First, although the primitive form was the last form standing after repeated mechanical division, Haüy could still impose a mathematical division that permitted the six forms characterizing his classification scheme to be reduced to just three. These he called integrant molecules (*molécules intégrantes*). Second, in order to work with only one shape (the parallelepiped) Haüy posited a yet more fundamental kind of unit, the subtractive molecules (*molécules soustractives*). For example, two triangular prisms make up a parallelepiped, six tetrahedra a rhombohedron, and so on. This move, Haüy believed, conferred greater generality on his theory. For a given crystal then, Haüy could determine the primitive and then the integrant molecule and then, working from the angles of inclination of the cleavage faces, calculate various ratios to generate the plane and interfacial angles of the integrant molecule.

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[20] This is reminiscent of the situation that led Newton to say "hypotheses non fingo." The absence of any theory of layering did not prevent Haüy from making symmetry inferences, just as the absence of any theory of action-at-a-distance did not prevent Newton from making inferences about planetary motion.

But the layering pattern had to be postulated too. As Burke explains:

> Every crystal face could be considered as having been built up by progressive addition of lamellae to it. Each lamella was thought to be formed of contiguous integrant or subtractive molecules and to have the thickness of one molecule. (94)

This can be seen in Figure 1 using Haüy's drawing of the simple case of a cube nucleus where the integrant molecules are also cubes. In this case, the crystal form is constructed on a cube nucleus with a decrement of two rows in width between OI and EA, II' and OO', and EO and E'O'; two rows in height between EO and AI, OI and O'I', OO' and EE'. A is the obscured corner of the square EOIA (*Traité* tome 5, Plate II).

Haüy believed that his method was complete. His overall positive heuristic was this: For a given substance, determine the primitive form of a crystal experimentally, then posit the laws of decrement, and compare the predicted crystal forms to those known. If there is not a good match, revise the primitive form or posited law of decrement.

Haüy's Classification Scheme

The classification scheme was also based on the primitive form of a crystal:

> [T]he primitive form of crystals of a certain species results as a nucleus from the cleavage of all the secondary forms. ("Haüy" 179)

After his lucky break, the accident with calcite, Haüy had his positive heuristic: he systematically shattered many other crystals to derive their primitive forms. In 1793 he

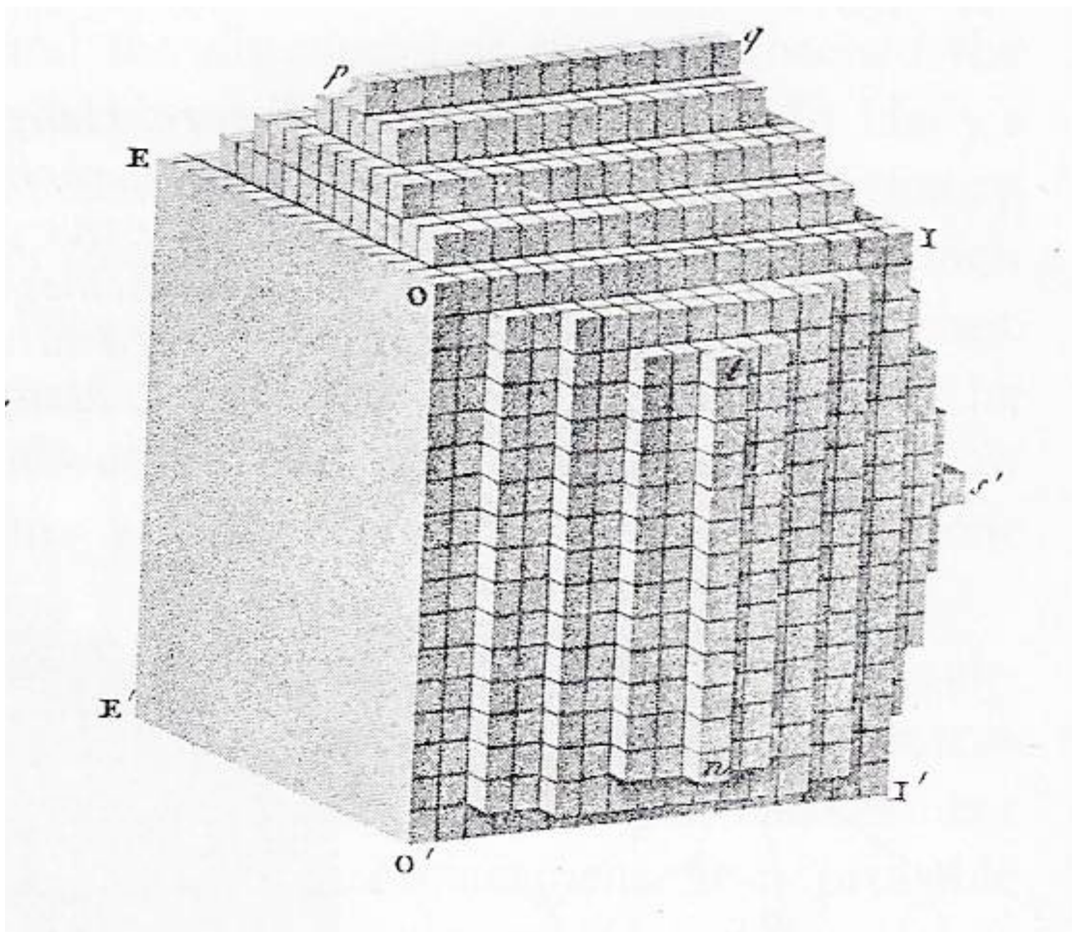

Figure 1 Dodecahedron with Pentagonal Faces

classified them according to six systems: parallelepiped, rhombic dodecahedron, hexagonal dipyramid, right hexagonal prism, octahedron, and tetrahedron.

Haüy's approach overcame the difficulties in the existing approach, that of Romé de l'Isle, mentioned earlier.[21] By seeing the respects in which Haüy did so and by seeing the difficulties his own approach developed, we will be able to appreciate why he needed to employ a specific concept of symmetry and the inferential work that it was required to do within his model.

At a minimum, Haüy's task was to rid classification of its arbitrariness. His method of repeated cleavage reduced the arbitrariness of the primitive form experimentally, and his explanatory model imposed constraints on the truncations and bevelings on the supposition that the new faces had to align with diagonal rows of integrant molecules. The angle of inclination therefore depends on a Law of Decrement, the number of molecules we skip as we slice through each layer. We see in Figure 2 the cross section in the *x-z* plane of a crystal formed out of cubic molecules, with its corner truncated by one molecule row by the plane AA' , two rows by BB', and three rows by CC'. (The planes are seen in cross-section as the lines AA', BB', and CC'.) One can show geometrically that the intercepts of the possible faces with the *z*-axis will be ratios of whole numbers. For a general three-dimensional crystal there will be a series of such ratios possible for each axis. Haüy derived this law (the Law of Rational Indices) from his explanatory

[21] Short histories of Romé de l'Isle's work can be found in Burke (62-77) and Hon and Goldstein (*From* Summetria 188-200).

model. Because part of the hard core of his model is the integrant molecule, fractional molecules are forbidden and therefore the intercepts must be ratios of integers. That of course has the advantage over Romé de l'Isle's model in that not all truncations would be permitted, a prediction that can be empirically checked.

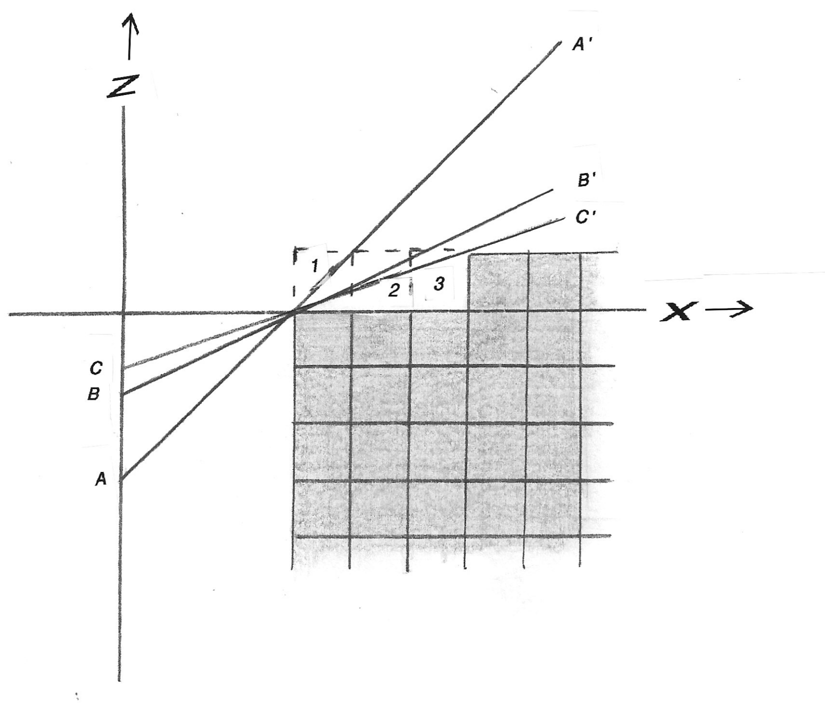

Figure 2 Cross-section of a Cubic Crystal Truncated by Planes

Although Haüy's model was empirically testable and could also reduce the arbitrariness of Romé de l'Isle's, his own Laws of Decrement, part of the hard core of his model, were also *ad hoc*. As no mechanism for crystal construction is presented it is not clear how the number of rows subtracted in each of the layers in his model is to be determined other than by matching them *ad hoc* to each observation. It might be one or two but there is no clear limit. This is not merely arbitrary; it leads to an unmanageable combinatorial explosion. With one or two rows subtracted, a primitive form might generate thousands of secondary forms, but with four it would be millions. Haüy had also found it necessary to postulate differential decrements in some cases — meaning that the decrement would one number of rows of molecules in one direction and another in the transverse direction (as is illustrated in Figure 1). With this degree of flexibility, his research program was degenerating. In an attempt to rein in this lawless profusion of decrements, Haüy turned to geometric symmetry.

Haüy's Use of Geometric Symmetry

Haüy was not the first to introduce symmetry into crystallography, but he applied it differently than Romé de l'Isle did because, unlike the latter, he was using it to relate external form to a (hypothesized) internal structure. He used it to relate the nucleus of a crystal and the various crystal forms that result when successive layers of molecules are added. He described symmetry (as if from the perspective of Plato's craftsperson) thus:

> … the manner in which Nature creates crystals is always obeying to the law of the greatest possible symmetry, in the sense that oppositely situated

> but corresponding parts are always equal in number, arrangement, and the form of their faces. (Haüy 1795, qtd. in Kubbinga 9).

This kind of symmetry inference seems to follow from the Principle of Sufficient Reason: if physical conditions at corresponding parts of the crystal are identical, there is no reason that the resulting geometrical shapes would not also be identical.

It is not before 1815 though that symmetry carries an important inferential load within Haüy's model. By that time Haüy could appreciate that he then had a plethora of laws of decrement and that these seemed arbitrary in the sense that they had to be selected to fit empirical data. So Haüy then subordinated these laws of decrement to a new law that he had postulated, the Law of Symmetry. This law, he supposed, was "remarkable for its generality and uniformity in the midst of the numerous modifications to which [the laws of decrement] are subject" (Haüy *Mémoire*, trans. Hon 196). The law would at least reduce the arbitrariness of the choice of possible decrements by restricting them to a *single* choice wherever physical conditions were the same — in practice, this means when the physical conditions are deemed to be equivalent wherever the geometric features of the crystal look the same.

This symmetry concept is geometric not aesthetic. As we saw, the prevailing concept was aesthetic, a concept that is more often used to characterize life, art, and architecture than inorganic nature; it referred and still refers to the balanced or fitting relationship of all the parts to the whole object and to each other, with connotations of beauty and elegance. But for Haüy, symmetry had to function in the *inferences* he needed to link the internal arrangement of the building blocks of his model to the external form of the crystal so modeled. These inferences included the identification and classification of the external forms that were possible as well as quantitative predictions about crystal faces and their planar and interfacial angles. Gabriel Delafosse (1796-1878), who was Haüy's student, described this geometric sense of symmetry:

> A whole is symmetric when it manifests a particular regular building plan which ordains the arrangement of the composing parts, a condition that implies that among those parts there are some that repeat themselves various times, maintaining in the process the same form and the same value, while occupying also similar positions with respect to a center or system of axes. (Delafosse 1840, qtd. Kubbinga 11)

This geometric symmetry was still metaphorically related to architecture, a planned building. But the parts of this building were then symmetric in the sense that they were *congruent* and occurred in *repeated* patterns (familiar in the decorative walls typical of Islamic architecture, say) rather than in the sense that they were *fitting* in shape and size or that they occurred in *balanced* relationships (familiar in the balanced room, door, and window layouts typical of Renaissance architecture, say).

Several features of Haüy's concept of symmetry are worth noting. First, it is related to Legendre's concept of symmetry (see §4.5) only in the sense that both crystallography and solid geometry treat three-dimensional space. But Legendre's definition concerns the *relation* between two bodies that are equivalent whereas Haüy's concerns a *property* of the whole object and is part of his classification scheme for crystal objects. Moreover, there is no evidence of any direct influence. Second, Haüy's symmetry was implicitly group-theoretic (see Scholz 111) in that it dealt with congruence relations that can be codified as such in Group Theory. But his work was driven by scientific concerns from the bottom up and in any case predated the insights of Galois by 15 years. Last, Haüy applies his law of symmetry in a modern way as a constraint on other laws. Symmetry principles do not for him uniquely define the laws of decrement but they do constrain them.

Haüy's Initially Progressive Research Program

I evaluate the progressiveness of the problemshift from the predominantly aesthetic concept of symmetry (used in the pre-scientific crystallography of his predecessors, the most proximate of whom was Romé de l'Isle) to the geometric concept of symmetry (used in Haüy's molecularist theory of crystals). As shown below, that problemshift was theoretically progressive at the time in the sense that Haüy's approach had an 'excess empirical content' its predecessor lacked; but it was ultimately superseded by an even more progressive approach, the algebraic concept of symmetry embedded in the crystal model and classification scheme of the German Dynamist School.

Theoretical Progressiveness

To show the theoretical progressiveness of this problemshift, I describe two features of Haüy's research program. The first is his 'hard core' molecular theory, in which he employed a concept of geometric symmetry in an explanatory model and classification scheme; along with the 'protective belt' used to defend it. The second is the content and inferential capacity that was surplus to what was required to account for known crystal facts and laws.

The hard core, a.k.a. ‘negative heuristic,’ of Haüy’s research program, is what defines it. In this program, crystals comprise integrant molecules of fixed chemical composition structured in one of several identifiable primitive forms that are determined experimentally through a process of repeated cleavage and by mathematical subdivision of that form. The external form of a crystal will thus be determined by its internal structure, i.e., by the shape of the integrant molecules and the way they are set down in layers on an initial nucleus. Crystals are regarded as aggregates of integrant molecules layered according to ‘laws of decrement’ that stipulate the whole number of rows by which each layer differs from the layer beneath it. Haüy subordinated those laws of decrement to a law of symmetry, a geometric symmetry that required all congruent and similarly positioned crystal faces to be treated the same way.

The research policy, a.k.a. the ‘positive heuristic,’ of Haüy’s research program includes the protective belt, that is, various suggestions about how elements of the theory other than those in the hard core may be modified or refuted in order to protect that hard core. For example:

> Since the values of the facial and interfacial angles which Haüy calculated for the varieties of calcite and other crystalline substance were in general agreement with the measurements of the contact goniometer on actual crystals, Haüy could … proceed confidently with the extension of his theory. (Burke 90)

In other words, even though calculated and measured angles differed somewhat (as they did on the obtuse facial angle on Iceland spar), Haüy’s general theory of molecules and decrements could survive — as long as that difference was more or less within experimental error. Here is another example:

> If the trial of many laws of decrement did not establish the required face of the secondary form with any degree of accuracy, then the integrant molecule required further investigation. The experimental part of Haüy's theory, them, was the establishment of the shapes of the integrant molecule and the primitive form and the application of the correct laws of decrement in order to develop the secondary form. (Burke 102)

In other words, if the observed external form of a crystal could not be matched to that predicted on the basis of the hypothesized primitive form of the integrant molecule, no matter what whole-number decrement laws we employ, we do not have to despair of our hard core. We can guess a new primitive form and start again.

The research program would remain a progressive one for as long as the adjustments under this positive heuristic are principled, but would become a degenerating one if the required adjustments were *ad hoc*. In terms of the examples cited above, Haüy could rely on the 'experimental error' defense in his day because of the limitations of the contact goniometer then in common use, but his theory came under increasing pressure once the more accurate measurements of the reflecting goniometer became available. And, although there is some flexibility in the choice of primitive form, that choice is constrained by Haüy's hard core assumption that the integrant molecule takes the form either of the crystal itself after repeated cleavage or of a further mathematical subdivision of that form, and cannot be just any old shape.

Initially, Haüy's research program was theoretically progressive, as we can see from the inferences we can make in it. First, structure. Haüy had shifted the problem from one of external form to one that concerned the *relation* between external form and a hypothetical internal structure. This is general enough for one to contemplate crystal structures other than the ones he was initially concerned with; to make predictions about possible crystal forms, including (perhaps) ones not yet observed; and to account for existing empirical laws, such as the law of constancy of interfacial angles. Second, discontinuity. Different ways of layering the same integrant molecules will result in different inclinations of the crystal face. Those angles of inclination will only take on certain discrete values though because they depend on the fact that only whole numbers of rows of integrant molecules can be added to or left off a given layer; any observed inclinations that are only compatible with fractional numbers of rows would be refutations of the hard core. Third, predicted existence. Some crystal forms may not have been observed in nature yet because the conditions for their crystallization were not met. But if these forms can be deduced by applying the laws of decrement to primitive forms already known to exist they would constitute a testable prediction.

Empirical Progressiveness

Haüy's program was also empirically progressive, insofar as there was corroboration of these inferences. Corroboration on structure came early:

> The main argument, comprehensibly, was the correspondence between theory and practice: the outcomes of Haüy's calculations of interfacial

> angles of his specially made beech models indeed neatly lined up with those measured from the pyrite crystals in his collection. (Kubbinga 4)

His work on another crystal, calcite, was particularly impressive: Postulating a nucleus in the shape of a parallelepiped (the primitive form he found empirically in calcite), Haüy had little difficulty to reconstruct the other crystal varieties; and by calculating various angles (using only plane trigonometry) he could show that the form of the integrant molecule for calcite was the same as that for Iceland spar, another form of calcium carbonate. His program could also show that beryl and emerald were actually the same species and that the various zeolites, which had previously been regarded as variants of one mineral species, were actually different minerals (Schuh 274). Corroboration on discontinuity was a little weaker though. On the one hand there was corroboration of Haüy's own Law of Rational Intercepts, now deducible as a consequence of the decrements used in his model. That meant that even crystallographers who had rejected his molecularism (such as the German Dynamists) still had to accept it as an empirical finding. Helpfully, most of the intercept ratios were simply expressed as ratios, such as 1:∞, 1:2, 2:3, 3:1, 1:3, etc.). But quite a few were not simple. That mattered; because large-number ratios could not always be measured accurately, even a century later, that made the matching seem very *ad hoc*.

> Finding that indices of crystal faces are often very large numbers a few authors … express the opinion that the law of rational indices has no meaning. For of course if we take the indices large enough any plane can be expressed by whole numbers. It is manifestly impossible to prove by

> direct measurement that the indices of all crystal faces are rational, for measurements are subject to certain errors, the measured angle rarely ever coinciding with the theoretical angle. (Rogers 108)

This issue is now moot since the intercepts, which are generally small whole-number ratios, are understood in terms of lattice theory and confirmed by techniques that were not available to Haüy.

Haüy's Degenerating Research Program

Although Haüy's research program achieved some notable successes, it began to degenerate and was eventually abandoned. While it did account for some empirical laws, such as the Law of Rational Indices, after a while Haüy's model was no longer theoretically progressive. For instance, it did not make any testable suggestions about the mechanisms behind hard core assumptions like layering and its Laws of Decrement. Nor did it in fact open the way to going beyond crystal shape to other physical properties or beyond crystallography to any other scientific field. Initially it seemed promising since, as Haüy's student Delafosse claimed, symmetry principles seemed important in other disciplines too — like zoology and botany — where it was also necessary to treat the relationship between individuals and aggregates (Kubbinga 12). Nevertheless, Haüy's research program was degenerating in the important sense that it required a profusion of new concepts and free parameters in order to keep on working.

We can see how Haüy's program became ever more *ad hoc* (and see how he attempted to rescue it by using symmetry principles) by tracing his solution to one of the three main problems of crystallography: the classification problem. Crystals in Haüy's time were identified as polyhedra (solid bodies bounded by plane faces). While the number of shapes is vast, not every shape is possible. Some variants were 'accidental,' others 'substantial.' A crystallography research program has to produce a scientific taxonomy, one that would at least determine what, if anything, underlies that riot of shapes; it is a quest for the specific invariants that can undergird a taxonomy. Haüy shifted the problem of categorizing crystals from one based on their *external* characteristics (generally favored by mineralogists) to one of explaining why they have the forms they do on the basis of hypothesized *internal* structures. In short, he claimed that small, identical, unobservable building blocks of a given shape aggregate in alternate, lawlike ways to construct the variety of crystal forms we observe for each type of crystal substance. The hard core of his program, as it relates to classification, had three components:

- The form of the building block, namely the integrant molecule. The form of the integrant molecule was postulated on the basis of the shape that the crystal took after repeated cleavage; that shape could be noted and the facial and interfacial angles measured.
- The patterns of aggregation, namely the laws of decrement. The laws of decrement were postulated to fit the observed crystal form, subject to the restriction that fractional decrements are forbidden.
- The fundamental unit of classification, the crystal species. The crystal species was the integrant molecule; while chemical composition determined broad mineral classes, it

was the form of the integrant molecule that had the specificity and invariance to define crystal species.

All three components of the hard core ultimately became untenable.

Form of the Integrant Molecule

Because the forms and patterns could be calibrated to fit each crystal observation, the research program was for this reason alone *ad hoc*. Haüy needed a principled way to restrict the shapes and patterns in order to have a testable hypothesis of crystal form. Lacking any empirical mechanism for the shape or aggregation behavior of his molecules, he resorted to *a priori* reasoning by reverting to the earlier (aesthetic) concept of symmetry.

Aesthetic symmetry, the principle that the parts of the whole be elegantly proportioned, was one way that Haüy had to limit the shape of the integrant molecules. "To Haüy," Burke suggests,

> nature had formed crystalline matter in accordance with the principles of simple arithmetic and geometry; we should not attempt to complicate matters once these simple relationships had been established. (92)

In particular, Haüy believed that the diagonals of the parallelogram on a crystal face should be in the ratio of square roots of integers and used this assumption "to derive the value of the interfacial angles, and consequently, the shape of the integrant molecules of those substances in which cleavage was absent or practically so" (Burke 92), That is to say, the principle, if true, would have a quite general capacity to limit the arbitrariness of the inputs to his model. We see this idea in action when, like Haüy, one measures the facial and interfacial angles on the rhombic faces of Iceland spar crystals and thence calculates two 'interesting' numbers: the inclination of the faces to the vertical (45°) and the ratio of the diagonals (√3:√2).

Embarrassingly, Haüy seems to have elevated his principle of aesthetic symmetry to the hard core of his research program and thus had to use his protective belt, i.e., the error margins of observation and experiment, to defend it. As wryly noted by a contemporary British crystallographer in 1819, Haüy was "disposed to regard generally the disagreement of an observed measurement … rather as an error of observation than a correction of his theoretic determination" (Brooke 454).

That protective belt maneuver came under great pressure in the years after 1809, when the reflecting goniometer was perfected, because experimental techniques became so much more precise. At the time, those techniques "appear[ed] to have excited a degree of anxiety in the mind of the Abbé lest his theory, which had availed itself only of the common goniometer, should suffer from any disrepute attaching to that instrument" (Brooke 454). In fact, meticulous measurement of those 'interesting' parameters of Iceland spar then showed that the actual inclination angle was an 'inelegant' 45°23' and the closest square-root of whole numbers ratio was a very 'unsimple' √111:√73 (Burke 92).[22] Other measurements reported around the same time delivered the same message:

> The well-known error to which an adherence to his principle of ideal simplicity [Haüy's use of aesthetic symmetry to limit the arbitrariness of his laws of decrement] has led this philosopher [Haüy] in his

[22] These values are quite close to those accepted now.

> determination of the primary form of carbonate of lime amounts to 37 minutes of a degree; and as he has assigned to the magnesian and ferriferous carbonates the same angle as to the simple carbonate, the error with regard to the these is still greater … (Brooke 454)

Laws of Decrement

Institut de France, in an otherwise glowing report to Napoleon on the state of French physical and mathematical sciences in 1810, lamented that in some ways Haüy's research program was quite arbitrary. It noted in particular the arbitrary laws of decrement he had to assume:

> Quant à la cause qui détermine dans chaque variété telle loi de décroissement plutôt que telle autre, elle est encore couverte d'un voile épais. (Cuvier 17)
>
> (The cause that determines for each variety one law of decrement rather than another is still covered by a thick veil. My translation.)

Geometric symmetry, the principle that parts that are geometrically congruent develop in equivalent ways, would at least constrain the Laws of Decrement to apply equally to all congruent faces of a crystal, even if it could not account for them. In his later work, five years after the *Intitut*'s report, Haüy codified his geometric constraint as the Law of Symmetry, which would subordinate his Laws of Decrements. It is not clear whether Haüy ever systematically demonstrated the operation of this law in any particular case, but given the other difficulties of his program that became moot.

Crystal Species

Finally, Haüy's research program was confronted by new discoveries that contradicted his relegation of chemical composition to a secondary status:

> There is a characteristic that is much more reliable and more suitable, because of its invariability, to serve as the focus for different bodies belonging to the same species. This is the exact form of the integrant molecule, because this form persists unaltered in spite of any cause that may make other characters vary …(Haüy, Vol. 1, p.156; trans. Emerton 270)

Haüy goes on to define a species as a collection of bodies that are composed of the same integrant molecules, composed of the same elements combined in the same proportions (162). It is in this context that we must read the discovery of isomorphism, polymorphism, and physical phenomena like pyroelectricity as serious rebuttals of his program. Eilhard Mitscherlich (1794-1863) showed in 1819 that different salts can crystallize in the same form (isomorphism). This undercuts the claim that the form of the integrant molecule is *specific* to the substance. In 1822 he went on to demonstrate comprehensively another phenomenon that had been understood only vaguely before, that the same substance can crystallize in more than one form (polymorphism). That undercuts the claim of *invariability* because this polymorphism does not refer to the different crystal shapes that might result from alternate laws of decrement using the invariable integrant molecule, but to those that result from building with integrant molecules that have another form. Then there were discoveries of physical effects in crystals that defied easy explanation in terms of geometric form at all — such as the generation of electricity in some crystals when heated (pyroelectricity) and optical effects like double refraction. These suggested that there are other features that might function as the specific invariants we need for crystal classification. One could (and Haüy did) make use of protective belt defenses in these cases — such as that the crystals of different salts are very similar to but not exactly the same as the ones to which they are allegedly isomorphic; that polymorphism results from trace contamination that makes the crystal substances in question not technically identical; or that the physical effects could nevertheless be related to some aspect of the form of the integrant molecule. But with repeated experiments and continuing discoveries these defenses also became untenable. It is against that background of failure that we need to view the developments in crystallography that followed.

4.4 Algebraic Symmetry

Algebraic symmetry, as I employ the expression here, refers to the property of objects (such as crystals) to appear completely unchanged when the conditions of observing have been transformed in certain specified ways. At the beginning of the nineteenth century, the symmetry of this kind that was most commonly understood was the reflection symmetry, often expressed in architecture and regarded as aesthetically positive. In this case, the right-hand side of a building is the image of the left-hand side as it would appear in a mirror whose plane bisects the building. Reflection in that particular plane is a 'transformation' that leaves the image of the whole object 'invariant.' Rotation was also understood as a transformation. For example, if observers walked around a perfect snowflake placed horizontally on the laboratory bench, their perspective is rotated about a vertical axis through the center of the snowflake; returning to the start position of course leaves the appearance invariant but, more interestingly, so too does rotating our point of view by only 60°, a sixth of a full circle of rotation, because the snowflake displays sixfold symmetry. Inversion is the last of the symmetry transformations that is commonly understood. This is associated intuitively with the center of symmetry. An object has such a center if every point on its surface is the same distance from this point as the corresponding point on the surface on the line joining them all. A sphere is such an object, and in the world of crystals so too are many (but not all) polyhedra. The cube is one that is. If the image of the whole object is inverted through the center, its 'inversion point,' it remains unchanged. Symmetries like these are properties of the whole object, which can then be characterized in terms of its inversion point, rotation axes, and reflection planes (if it has any). Geometric symmetry, by contrast, refers to the congruence, or geometric equivalence, of parts of an object; aesthetic symmetry refers to the fitting, elegant, simple, or otherwise pleasing proportions of its various parts, many of which will not be equivalent to one another other at all, but will be shaped and sized in appropriate relationships.

Weiss, who was the most important early figure in the German school of crystallography, introduced the notion of algebraic symmetry into the field. He did so at the time Haüy's research program was degenerating in the ways set out above — and despite Haüy's own efforts to shore up his program by using both aesthetic and geometric concepts of symmetry to minimize the number of brute facts and arbitrary parameters. In fact Weiss introduced this symmetry in the notes he appended to his translation of Haüy's *Treatise*, the first German translation, one that he completed in 1810 after six years of labor. Weiss though employed an algebraic notion of symmetry and made it the central feature of his account right from the beginning.

For expository reasons, we may date the heyday of algebraic symmetry conventionally as starting around 1815, when Haüy published his Law of Symmetry, and ending around 1850, when Auguste Bravais (1811-1895) completed the mathematization that Weiss had begun. The end date does not indicate that the algebraic concept was superseded but only that considerations of another kind of symmetry, which I will term 'physical symmetry,' became dominant.

The Problem Situation in Crystallography circa 1815

To appreciate the tasks facing crystallography around 1815 we also need to understand what was happening in related disciplines. Crystallography was still emerging from mineralogy; it concerned many of the same objects that mineralogists studied and many of its practitioners were, like Haüy and Weiss, mineralogists themselves. It was also influenced by chemistry and natural philosophy, insofar as those disciplines also made claims about the constitution of matter.

Mineralogy continued as a separate discipline from crystallography, addressing somewhat different questions about crystals. The distinction was not always clear and mineralogy continued to exert a strong influence on crystallographical thought. In particular, there was still a preference for morphological approaches over structural ones, that is, for accounts rooted in directly observable external forms rather than on unobservable hypothetical components and configurations. For Abraham Gottlob Werner (1750-1817), the external characteristics of a mineral were enough for mineralogy's primary task of identification (Burke 59). Even a century later, crystallography was seen by mineralogists as being far too much of a 'mathematical science,' given that what was really needed was an

> observational study with the application of a few simple rules that will enable the prospector and laboratory student to determine the crystalline form with sufficient accuracy for practical purposes in the field or laboratory. (Wadsworth v)

Chemistry was a burgeoning science and was, it must be said, increasingly well disposed toward molecular theories. However, Haüy's integrant molecule was not just the chemical molecule as we know it today nor just the unit cell of a crystal lattice as in modern crystallography, but somehow both. The claim was that it could identify the crystal substance it comprised because it was both specific and invariant— when in fact it was increasingly evident it was neither, especially after the discovery of isomorphism and polymorphism.

Natural philosophy, insofar as it affected Weiss and the German school of crystallography in general, took the form of *Naturphilosophie*, which was unsympathetic to molecular theories. Weiss subscribed instead to dynamism, holding that matter resulted from the balance of attractive and repulsive forces and that it was infinitely divisible. This philosophical outlook was important because it had a respectable pedigree, including the views of Leibniz and Kant, and because it would have predisposed one to the kind of problemshift that Weiss proposed for the study of crystals.

The problem situation that Weiss faced thus required him to address the problems of crystallography, principally those of classification, in a way that neither presupposed molecularism nor degenerated into arbitrary parameters the way Haüy's had.

One can discern two problemshifts in the algebraic phase of crystallography initiated by Weiss. The first problemshift was Weiss's retraction of the problemshift that seemed to have landed Haüy into trouble: focusing on the relationship between external form and internal structure. Haüy had needed to posit so many hypothetical shapes and patterns to make his explanatory model work. Weiss instead moved back to a morphological approach: focusing only on external form. This time though crystal shapes were to be described and classified in terms of new elements, crystallographic axes of symmetry and algebraic symmetry. The second problemshift occurred around 1850 with a reversion to focusing on the relationship between external form and internal structure.

The First Problemshift: Morphological Approach and Axes of Symmetry

The morphological approach was one that focused on what one actually saw -- namely, the form of the observable, macroscopic, crystal — rather than on what one had hitherto just hypothesized -- namely, the form of the unobservable, microscopic, structural units and the way they were arranged. It helped to avoid the arbitrary decrement patterns and molecular shapes of the molecular theory, and to eschew the use of integrant molecules, which the discovery of isomorphism and polymorphism had undermined. It was not really surprising that Weiss had chosen this approach, as he had been a student of the German founder of mineralogical science, Abraham Gottlob Werner (1750-1817). Mineralogists are professionally concerned with identifying minerals on the basis of external form and "[p]upils of Werner [had become] the guardians of mineralogy in the early 19th century" (Schuh 211).

One can conceive of the problemshift as a move from geometric to algebraic symmetry. Using geometric symmetry, what one deems to be equivalent are particular faces and edges that pertain to the crystal *object*; using algebraic symmetry, what one deems to be equivalent are particular perspectives on the crystal that pertain to the observing *subject*.

Crystallographic axes were to be the basis of the classification of external form — rather than the primitive forms of any structural units. Axes are vectors (directed lines) with respect to which one can describe the symmetries of crystal properties. Weiss would use axes with a specified polarity (one end being conventionally 'positive,' the other 'negative') to incorporate descriptions of physical phenomena about which Haüy's model was silent. The phenomena that Haüy ignored were those that occur along lines in a preferred direction, such as pyroelectricity. (A pyroelectric crystal is one that, if uniformly heated or cooled, will develop an electric potential in a favored direction in the crystal, one side regarded conventionally as 'positive' and the opposite side as 'negative.') Haüy had been aware of these effects, which contradicted his model, but just ignored them. In his 1815 memoir on the law of symmetry, he

> consciously excludes certain crystals, among others boracite and the tourmalines, a group of silicates which, when heated, charge themselves

> electrically, a process showing the presence of an 'axis' linking the oppositely charged parts of the crystal. (Kubbinga 9)

Physical effects like this are hardly exceptional though — Schuh catalogs many types, ranging through optical, thermal, mechanical, and electrical (120ff). One striking effect is the optical one known as 'double refraction' or 'birefringence.' This is the property of a crystal to split a light ray into two rays, with the angle between those rays depending on the viewing angle and diminishing to zero as one's line of sight gets closer to a unique line, dubbed the 'axis of double refraction.' The effect was discovered way back in 1669 in Iceland spar, the much-studied variety of calcite on which Haüy had worked as well (Schuh 200). Other examples include thermal expansion (since heated crystals typically expand at different rates along their axes), elasticity, hardness, thermal and electrical conductivity, and piezoelectricity (the generation of an electrical potential through a change of pressure). Weiss applied his 'dynamist' model of attractive and repulsive forces to these effects and suggested that it was the crystallographic axes and their polarities that were fundamental.

Weiss's Crystal Model

Weiss had a qualitative model of the constitution of matter, and therefore of crystals. This was based on polar theory, which had been incorporated into *Naturphilosophie*. He set out his views in a lengthy appendix to his 1804 translation of the first volume of Haüy's *Treatise* (Burke 151). There he proclaims his goal of developing a model that would show how crystallization results from the regular pattern of interior forces. This was not a molecularist account of forces between atoms that comprise molecules but one of forces that generate matter itself. Forces are unobservable but, as in Haüy's model, we may see their effects by the crystal faces they generate as secondary consequences and from cleavage along lines of weakness. "Weiss's investigations led him to conclude that the whole system of crystal forces always contains three spatially extended main forces, from which all other internal forces can be derived by composition" (Scholz, "Influence" 38). This account did not give rise to any quantitative scientific model, although it was qualitatively consistent with the observed directional effects in crystals, such as cleavage. By 1811 though, in his dissertation, Weiss was no longer making any specific use of his qualitative model.

Nevertheless the symmetry concept that Weiss introduced into crystallography has proved unquestionably useful for inquiry ever since. At first glance this seems odd, because the theory of matter he held had never outgrown its metaphysical origins but had remained speculative; it was moreover curiously out of step with the ascendency of molecularist theories of matter in his time — not to mention ours. As it turns out, his theory of matter did not retard crystallography because the details about how those attractive and repulsive forces arose played no direct role in addressing the main crystallographic problem, that of classification. Only the symmetries played any role and because Weiss's heuristic identified them directly, that was sufficient. This was unlike Haüy's case, as it was his crystal model that explained the observed forms. What was really important was that the concept of symmetry Weiss introduced made certain material inferences possible without requiring a commitment to any specific theory of matter, molecular or otherwise. That gave Weiss's approach a generality that Haüy's lacked due to its dependence on a particular model of crystal constitution.

Weiss's Classification Scheme

The defining problem of crystallography was that of classification, that of finding specific invariants that uniquely identify a crystal species despite the vast number of accidental and secondary forms. Weiss believed that the source of Haüy's failure lay in molecularism: one could not assign a crystal of a given external form to a class on the basis of the form of its integrant molecule if that form was neither specific to the substance nor invariant. Rather than showing how, roughly speaking, big objects of particular observed shapes were built out of little objects possessing other particular shapes, Weiss aimed to show how observed forms could be generated from a set of their symmetries.

The basic units of Weiss's scheme, axes, could be observed directly. In 1809 he wrote:

> An axis … is a line that dominates the whole crystal form and around which all parts are uniformly arranged. (Weiss 42; trans. Kubbinga 14)

He argued that there were either three orthogonal axes or four (where three of those are orthogonal to the fourth), and that these could be determined by inspection. His system had an immediacy that Haüy's lacked, and was also easier to use:

> Haüy's followers admitted that the German method had one advantage: it was much easier and more effective in teaching to give a dogmatic exposition of principles of crystallography to students whose practical

> experience was limited; the German method was easier to learn. (Burke 166)

While crystallography occupied itself more and more with the mathematics of classification, mineralogy was where the empirical work of classification was done — by measuring interfacial angles as usual, but now also determining the dimensions of the crystal axes and judging which external forms were related. One experimental advantage was that one could also use physical symmetries other than external form when it was expedient to do so; axes of double refraction, for example, are generally easier to determine than axes of crystal shape.

Symmetry, specifically that associated with axes of rotation, was to be primary; the forms of crystal faces could be derived from them. The positive heuristic was: first determine the crystal axes, generally three and sometimes four in number, their dimensions; directionalities (if any); and their symmetries. Then, on the polar theory at least, one could rely on the fact that there would be counterbalancing forces, vectors, that would be acting along those axis directions. Crystal planes, Weiss thought, would form perpendicular to those forces. Lines where those planes happened to intersect other planes would determine the actual faces and their shapes. Weiss identified seven systems in which all crystal shapes could be classified in this manner.

Weiss must take the credit for the original idea of using algebraic symmetry and for establishing a crystallographic research program on that basis. Although Weiss himself did little to develop the program further, other members of the German school understood that it was theoretically very progressive — both ripe for mathematization and capable of producing a complete classification scheme using just a few elementary symmetry operations. Two leading figures, Moritz Ludwig Frankenheim (1801-1869) and Johan Friedrich Christian Hessel (1796-1872), for example,

> realized that, notwithstanding the seemingly endless disparity, there are limits as to the geometry of crystals, and that a rigorously strict deduction of the distinct possibilities in terms of symmetry was a feasible enterprise. (Kubbinga 15)

In other words, since the task of crystallography had been defined mathematically in terms of symmetry operations, the classification scheme could be completed deductively.

The hard core of Weiss's research program can be ascertained from his actions and writings and from contemporary commentary.

- First, it included a commitment to mathematization. Even the title of his 1807 dissertation, *Dissertatio de Indagando formarum crystallinarum charactere geometrico principali* ("Investigation into the Principal Geometrical Characteristics of Crystal Form"), suggests as much. The contrast he drew there between his system and Haüy's was not lost on his French translator, who noted in 1811:

> Il pense que *tous les cristaux ont un axe*, et que l'axe étant dans toute forme géométrique une ligne unique, principale et dominante, le *caractère géométrique d'un cristal doit être fondé sur des [éléments] ayant un rapport direct avec l'axe*. (Brochant de Villiers 350)
>
> He thinks that *all crystals have an axis*, and that the axis in all geometrical forms is a single line, principal and dominant, the *geometric character of a*

> *crystal must be based on elements directly related to the axis*.(My translation.)

Once the problem had been specified in terms of finding crystallographic axes and relating other features to them, the way was open to mathematization.

- Second, Weiss was committed to the hypothesis that symmetries were the fundamental elements in the classification and to the belief (inherited from *Naturphilosophie*) that crystal systems derived in this way reflected the balance of actual forces in the world, and were thus what we would now term 'natural kinds.' That belief would have legitimized the use of physical phenomena other than observable external form to experimentally determine the symmetries of crystal substances and the further application of those symmetries to physical phenomena other than the ones used to make those determinations. "It should be emphasized, " Burke tells us

> that Weiss did not believe the systems or subdivisions he proposed were mere geometrical constructs. As the title of his memoir[23] indicated, these were natural divisions. The variables that characterized each division and subdivision depended on the operation of natural processes. (Burke 159)

[23] This was the 1815 memoir in which Weiss presented his ideas to the Academy of Berlin. It was entitled "Uebersichtliche Darstellung des verschiedenen natürlichen Abteilungen der Kristallisations-systeme" ("Clear Presentation of the Different Natural Divisions of Crystal Systems").

- Third, although it included forces in a general way, Weiss's hard core did not actually include any specific metaphysical ideas about them. In his dissertation, for example, he merely noted that crystal forms were the necessary result of the generating forces.

Weiss's immediate successors in the classification task -- Frederick Mohs (1773-1839), Frankenheim, and Hessel – had remained open to ideas about inner structure and later re-admitted it. We can therefore describe their choices by saying that the main hard core assumption by then was the mathematics of external appearances, crystal morphology, rather than any metaphysical commitment to polar theory, since polar theorists had previously been opposed to structural ideas.

Weiss's Progressive Research Program

Symmetry effectively became the subject of its own research program. Weiss and his successors had so thoroughly mathematized crystallography that it became possible to make many discoveries deductively, once the 'correct' mathematical representation of mathematical objects in a three-dimensional space had been discovered. Clearly, the discipline was theoretically progressive; wherever a heuristic counter-example was found, one just needed the 'right' way to generalize the original insight of Weiss or to remove a condition that was unduly restrictive.

In the initial phases of this research, the protective belt was very protective:

> The morphological study of crystals in the 19th century tended to be limited to descriptions of ideally formed crystalline forms. This was particularly true of the German school headed by Weiss and Mohs. However, attempts to translate from idealized, theoretical models to

> natural crystals, with all their complications and imperfections, was not easy. In fact, for a long period such comparisons, which usually conflicted with the models developed by the morphologists were not attempted. It was only much later [that] the value of comparisons between theory and nature was recognized that the physical study of real crystals was intensified. (Schuh 210)

In other words, apart from any defense along the lines of 'experimental error,' the initial symmetry research program did not concern itself with any real-world crystals other than those found perfectly formed or grown that way under controlled conditions. The research program was conceived, for all intents and purposes, as one in the applied mathematics of objects (of whatever physical type) in three-dimensional space and could be justifiably shielded in its infancy from the vicissitudes of empirical data. Although this was a very fruitful era of research, discomfiting empirical results could not be ignored forever. For example, how does one account for odd geometric phenomena, such as the appearance of crystals bound together as symmetrical twins? And, of course, if symmetry is a mathematical concept, what warrants symmetry inferences about *physical* phenomena?

The first phase of research was on extending the insights of Weiss; members of the German school mainly carried out this work. Weiss had originally considered crystallographic axes that were orthogonal. But by 1822 Mohs generalized this to the more useful case of axes at oblique angles, to derive the crystal systems (Burke 166; Schuh 207).

- Weiss had shown, by a semi-empirical method, that there were seven systems of crystal shapes. But by 1826, Frankenheim argued, after considering the possible symmetries, that it was sufficient to look for subsystems among Weiss's systems, arriving at a complete list of the 32 classes still used.
- Weiss had introduced the three-dimensional axis system. By 1829, Justus Günther Grassmann (1779-1852) introduced a type of three-dimensional vector analysis to best represent the system of forces within crystals within the dynamist tradition (Scholz, "Rise" 119-21; Scholz, "Influence" 40ff).
- Weiss had considered only axes, which define only rotational symmetries, but by 1830 Hessel had added planes of reflection and points of inversion as well. He could also show, through his own comprehensive *geometric* analysis of all the possible combinations of symmetry elements pertaining to external form, that every possible crystal shape can be matched to one of 32 unique sets of all those symmetry operations — although the resulting 32 classes of crystal could still be grouped by their characteristic shapes into six or seven crystal systems.[24] Hessel also made the interesting discovery that only 1-, 2-, 3-, 4-, and 6-fold symmetries would be found in a crystal.
- Weiss had restricted himself to morphology and considered only the symmetry of external form. But by 1835, Frankenheim had also considered the symmetries of inner structure. The dynamists were opposed to molecularism but not to the idea of inner structure itself; after all, they conceived matter as being constituted by forces between

[24] The hexagonal system is sometimes divided into two.

non-extended points. In any case, Frankenheim came up with the idea of a space-filling lattice of these points and showed mathematically that in three dimensions only 14 configurations of lattice points are possible.[25]

Strikingly, publication of this early theoretical work was not at all historically influential. Its results are certainly impressive and have stood the test of time, and the work of these scientists is generally included in rational reconstructions of the development of crystallography and cited as examples of theorizing inspired by a particular philosophy (dynamism). But Frankenheim's 1826 paper was "completely without influence" (Scholz, "Rise" 118); Grassmann's work influenced that of his son, Hermann Grassmann, on vector analysis (Scholz, "Influence" 40ff), but that vector formulation "was very different from the structure of the modern system" (Crowe 249); and Hessel's work "received no recognition among his contemporaries" (Schuh 230) and languished in obscurity until 1891("Hessel" 359). For any influence on the science of crystallography, we need to turn to the second problemshift.

The Second Problemshift: Return to Internal Structure

The research program became a degenerating one when dealing with physical properties other than shape. It had become increasingly evident that the symmetry of the external form could not alone account for the physical effects without arbitrary

[25] He actually claimed there were 15 but later analysis showed there was a mathematical error in his demonstration. The corrected version of his proof shows there are 14 (Schuh 230).

adjustments. The second problemshift addressed this by connecting studies of external form with symmetries characterizing internal structure.

This problemshift was, in effect, a rapprochement between the German dynamist approach and the French molecularist approach. The German school had already begun thinking about internal structure, at least on their own terms, as Frankenheim did. The French school had never given up on it, although Delafosse, a student of Haüy, had by 1840 given up on certain specific aspects of Haüy's molecularism, such as the idea of the integrant molecule being the chemical molecule; he conceded that the integrant molecule might be just the space belonging to a lattice point, with a space-filling shape, a unit cell, outlined by the lattice points. As such this model was not very different from the German one. The hard core of this joint model in effect replaced both 'molecules' and 'forces' with the relatively theory-free zone comprising a lattice that had three dimensions of periodicity.

This was theoretically progressive. From this new starting point, another burst of mathematical symmetry research was unleashed. In 1848 Bravais studied all the geometric forms that could be built from a regular array of lattice points, coming up with accounts of external form and cleavage planes in terms of the density of lattice points when viewed in different directions, and an account of the crystal systems (Burke 171; Schuh 230-31). Like Hessel, but apparently independently, he derived the 32 crystal classes (as a type of group known as 'point groups'). Like Frankenheim, he derived the 14 lattice configurations possible (as those that preserved the symmetry of the unit cell in a periodic lattice under the additional symmetry operation: translation). This work was highly mathematical, but the upshot was that symmetries of external form and other observed phenomena could be related to those of an internal (hypothesized) structure. That was a progressive move: it opened the door to making two-way inferences, i.e., inferring structure abductively from observations and then predicting new effects deductively from that structure.

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This concludes the last of three sections showing how the concept of symmetry has co-adapted with developments in crystallography. I now address a claim that challenges this empirical view.

4.5 An Alternative View: Mathematical Symmetry

I consider an objection to the thesis that symmetry warrants are material and based on co-adaptation, one that is expressed as a rival claim that the scientific concept of symmetry developed in mathematical research and was then transferred to the physical sciences. I analyze the three most plausible variants of this claim. Each is centered on a particular field of mathematics that is currently used in the physical sciences to describe symmetry operations: Solid Geometry, where this rival claim has been made explicitly; Group Theory, which is now regarded as the mathematical language of symmetry; and Vector Analysis, which was founded by mathematicians but honed by physicists for use in, among other matters, certain symmetry operations.

The Applicability of Mathematics

The applicability of mathematics to science itself has the attributes of a scientific research program. Hypotheses about which formalism is most applicable for a particular inquiry can be ‘corroborated’ by the empirical success of that inquiry — whether it is useful in inferences, convenient to use, further expandable, etc. Such arguments are never decisive; there is no ‘fatal flaw,’ like an internal contradiction, to close the discussion. (That may be why these mathematical discussions can be so vehement.)

The issue of the applicability of mathematics is not a new one. Since antiquity, social organization and political control have been important drivers of mathematical development. That does not address the issue of the foundations of any mathematics so developed — the source of any *a priori* demonstrative capacity it may have, say — but merely asserts that the wisdom of choosing any particular line of mathematical research from an infinite menu has to be evaluated against other criteria, such as whether the formalisms thereby developed prove useful in making subsequently corroborated material inferences in other domains like physics. This is not always the case, and no mathematics is self-evidently applicable.

Two-dimensional geometry has been applied since antiquity. Plane geometry, which analyzes figures on flat surfaces, is known as Euclidean. Its development was probably driven by the needs for land surveying where it has obvious utility. Spherical geometry, which analyzes two-dimensional figures on the surface of a sphere, is not Euclidean. Its development was needed for astronomy and navigation. Spherical trigonometry is the branch of this geometry that analyzes the angles and sides of the polygons constituting those surfaces.

In 1679, Leibniz foresaw what crystallographers later came to appreciate for keeping track of the symmetries of crystal form and structure: the need to develop a thorough-going three-dimensional geometry. Admittedly, the *volumes* of some three-dimensional structures had already been calculated, but what Leibniz was calling for was an analysis of 'situation,' one that goes beyond the expression of mere magnitude (as is done in standard algebra) to include position, angles, and direction. This turned out to be a far more complex extension of plane geometry than one might expect from just adding one more dimension. But although Leibniz never worked out these details himself, "he advanced far enough to be ranked as a conceptual forerunner of the first vectorial analysis" (Crowe 3). The quest for a useful way to represent three-dimensional space and to express the problems we need to solve there became a major focus of nineteenth century mathematics, and is present in all the mathematical research programmes relating to symmetry that are treated below.

Solid Geometry

Solid geometry is the geometry of three-dimensional space, which is clearly vital to crystallography and physics.

Solid geometry is important in the study of symmetry because it provides a way to represent forms in three-dimensional space. In particular, it can distinguish two classes of equivalence between paired objects: reflection symmetry, where the forms of the objects are mirror images of each other, and translation and rotation symmetries, where the objects can be moved and rotated to make them exactly superimposable. Stereochemistry, the study of the way atoms are arranged in the three-dimensional spatial structure of molecules, is an example of a scientific subfield that depends heavily on such distinctions.

The mathematical research programme in solid geometry was a progressive one. This was in no small way due to the contributions of Legendre, a highly regarded French mathematician of the revolutionary era. The progressive problemshift of his that most affected the study of symmetry was one that he introduced in 1794, his radically new concept of symmetry, one that is very close to the modern one. Legendre had been considering three-dimensional analogues of the two-dimensional concepts of similarity and equality that Euclid had used. He had been hoping thereby to describe and analyze solids, just as we had always been able to analyze figures in the plane.

This is no easy task. To take just one example, in 1758, as Lakatos notes, the great mathematician Leonhard Euler (1707-1783) identified a difficulty in the classification of polyhedra, the three-dimensional analogs of polygons. Polygons (plane figures bounded by straight lines) differ from polyhedra (solid bodies bounded by plane surfaces) in that plane figures are defined by their edges and the angles between them whereas solid figures are defined by their plane faces and the vertices (solid angles) between them, although they also have edges. It becomes clear that the number of faces alone is not enough to classify polyhedra (*Proofs and Refutations* 6). In response, Euler had developed an empirical formula that related the vertices, edges, and faces but it was Legendre who later offered the proof for the validity of Euler's formula.

Among other things, Legendre needed to come up with a definition of 'solid angle' (the angle formed between three intersecting planes, such as at the apex of a pyramid) and offered the following definition:

> Two equal solid angles which are formed (by the same plane angles) but in the inverse order will be called angles equal by symmetry, or simply symmetrical angles (citation and translation by Hon and Goldstein, *From* Summetria *to Symmetry* 2).

What was radical about this definition, according to Hon and Goldstein, is not so much what it says about solid angles but the implicit definition of symmetry, which was cast in terms of a mathematical operation of inversion. Informally, we can describe Legendre's accomplishment as the identification of two solid angles that are mirror images. One way two solid angles may be regarded as equivalent is where we can imagine one superimposed on the other exactly. But another way is where the same three planes (A, B, C) intersect but in the inverse order (A, C, B). There is no analogue for this in the plane, where just two lines intersect to form an angle. As a result, we could describe this conceptual change within mathematics quite well using a Lakatosian framework: the heuristic counter-example is the three-dimensional analog of an angle, about which Euclid was silent. Legendre could have defined solid angles in many different ways but the particular way he did helped the mathematical research programme to progress.

Hon and Goldstein make the empirical claim, in several places, that Legendre's mathematical definition drove scientific research programmes. In 2005 they write:

> [W]e investigate Legendre's work on solid geometry where he introduced a new definition of symmetry that, we claim, has served as the basis for the modern scientific concept of symmetry. We consider this new definition a conceptual revolution …

("Legendre's Revolution" 109).

At first glance this claim seems attractive — Legendre's definition incorporates a concept of symmetry that refers to a transformation (in this case, inversion) that leaves a property invariant (the solid angle). This mirrors the language used in current-day symmetry applications in the sciences.

There are, however, several reasons to doubt that Legendre's definition was a primary driver of the scientific concept of symmetry. First, although Legendre uses the term 'symmetry,' his main focus really is on the definition of a solid angle. Second, no mere definition seems capable of bringing about a revolution in an empirical science unless it is explicitly applied to the subject material and tested empirically. Third, and most serious, the historical evidence of any actual influence is lacking. Hon and Goldstein make the *post hoc* argument that "[t]he impact of Legendre's definition is … discerned in the quickening pace of usages of symmetry in the early years of the 19th century complete with new definitions" (*From* Summetria 49). But historiographical evidence is not presented. Legendre worked completely within a mathematical research programme and does not apply the symmetry concept to any physical object himself. If it had been applied by others at all we would certainly expect to see evidence of that in crystallography when, almost 20 years later, a concept of symmetry was applied. That occasion was Haüy's theory of 1815, the first scientific theory in crystallography, which posited a 'Law of Symmetry' about crystal structure — but which makes no reference to Legendre. Hon and Goldstein lament this lack: "Curiously," they say,

> Haüy does not refer to previous usage of symmetry in mathematics by Legendre, Lacroix, and Cauchy. Since all these Parisian scholars were connected in many ways, and sometimes even served on the same committee, it seems implausible that they did not know of each other's work. So one puzzle that will have to be solved in future investigations is the relationship of these early usages of symmetry in a scientific context ("Legendre's Revolution" 151-52).

Three years later, they offer this explanation:

> Although usages of symmetry by Legendre and Haüy suggest a connection — after all, both solid geometry and crystallography deal with three-dimensional figures — there is a great difference between the applications of the concept by these scholars. Legendre's concept is relational, namely, symmetrical bodies present a special kind of relation — equality by symmetry — which Legendre defined precisely and included thereafter in a deductive argument. By contrast, Haüy's concept of symmetry which formed part of his taxonomic apparatus, concerned the shape of the entire body of a single specific crystal, that is, the concept of a property, not a relation (*From* Summetria 63).

In other words, the concepts were different after all and so Legendre did not shape Haüy's scientific theorizing in any obvious way. In any case, Hon and Goldstein's 2008 study covered only the period from 1788 to 1815, so it did not include scientific work after Haüy's 1815 theory, such as the work of Pasteur or Curie. But they later noted that no such influence on the sciences had ever been recognized and, curiously, took that lack of recognition as itself a sign of influence:

> The fact that Legendre's contribution has not been recognized in books on symmetry in the sciences is a mark of success of the revolution he initiated. … What is amazing is Legendre's success to the degree that his role in this matter has been almost entirely forgotten (*Double-Face* 71).

In conclusion: it's unlikely that Legendre's definition was in any way responsible for the development of the symmetry concept used in the physical sciences.

Group Theory

Group theory is the study of groups, algebraic structures with particular abstract properties.[26] It was because solutions to some problems posed by classical algebra could not be solved that Galois and others devised the more abstract methods of Group Theory.

Group Theory is important for the study of symmetry because it has become the very language in which symmetries are classified and described. The use of Group Theory has become pervasive in twentieth-century science, particularly physics and chemistry.

The mathematical research programme in Group Theory was a progressive one. This was despite the fact that the impact of Galois' pioneering work, and that of others in

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[26] Abstract algebra is the study of abstract, axiomatic systems. It includes the study of abstract systems known as groups, rings and fields, which have been important in both mathematics and the sciences; linear algebra is sometimes included in this broad category as well.

this field, was initially quite slight; Kleiner describes algebra in the nineteenth century as "concrete by our standards" and "connected one way or another with real or complex numbers" (91). But the problemshift that Galois introduced has opened up new areas of mathematics and methods of proof.[27]

To determine what if any influence Group Theory (or any other branch of abstract algebra) had on the scientific research programmes of the nineteenth century, we need to look at *unreconstructed* accounts and histories of the sciences in this period. This is because Group Theory is now used so widely in the sciences that it is tempting to think that Group Theory itself was somehow responsible for the initial development and systematic use of the concept of symmetry there. But just in the field of physics alone, so much rational reconstruction has taken place, in the interest of providing a unified presentation of basic concepts, that the historical process of concept development has been obscured. (There are even transformation groups associated with scientists working well before Galois' time, such as Galileo!)

Group Theory had no influence on the formation of symmetry concepts in crystallography because those concepts had been developed, empirically, before Galois'

[27] For example, Galois himself was able to solve a problem that had bedeviled mathematics for 350 years, namely, whether quintic equations (those in the fifth power of the unknown) could always be solved in terms of mathematical expressions known as radicals. He solved it by exploiting certain symmetries associated with the equation, which could be expressed in terms of the properties of an abstract group known as the group of that equation.

breakthrough of 1830. Scholz, who is careful not to reconstruct the past in the light of our current understanding, reveals this in his account of the development of symmetry concepts in the fifteen years after the period considered by Hon and Goldstein (i.e., from the work of Haüy in 1815 through that of the German dynamists around 1830). He observes, *inter alia,* the gradual use of group concepts by crystallographers in this period. For example, he notes that Haüy had developed a systemic concept of symmetry which was, “if looked upon from an operational point of view, an implicitly group theoretic characterization of symmetry” (111) and notes that the classification by Weiss of the axial symmetries of crystals would be regarded as one of finite orthogonal groups “in today’s language” (109). Scholz also notes that Frankenheim, following Weiss’s work, had derived geometrically the 32 possible subsystems of crystals (known as the Crystal Classes), so that “from a group theoretic point of view, [Frankenheim] gave a complete enumeration of those finite orthogonal groups which arise as point symmetries in crystallography.” But Scholz cautions: “Of course, it was impossible for Frankenheim to use an explicit group concept in the algebraic sense. That was, as is well known, not yet even formed in algebra itself” (117).

By the close of the nineteenth century, crystallographers gradually became aware of group-theoretic methods. It wasn’t until 1884 that the formal methods of Group Theory were introduced to science when Bernhard Minnigerode (1837-1896) did so in crystallography. Even then they were not taken very seriously; his “novel mathematical methods” were regarded as complex and “disproportional to the simplicity of the problem” (Katzir, “Piezoelectricity” 87-88). A decade later, Curie refers to these methods in his 1894 paper (Castellani 323). But even though Curie was also aware of the work of Galois,[28] and may have known about Minnigerode's work, he does not refer to them in his paper.

In conclusion, it wasn't until the twentieth century that Group Theory (and abstract algebra more generally) had any major impact on the development of symmetry concepts used in the physical sciences. As Martin records:

> Although groups made their appearance in physics at the beginning of the nineteenth century, it was not until the detailed study of group representations in the 1920s which accompanied the developing quantum theory … that groups made their way into a large part of work-a-day physics. (30)

Vector Analysis

Vector analysis is the branch of mathematics that is concerned with mathematical operations on vector fields. A vector field is the assignment of a vector (a quantity having both magnitude and direction, like a velocity) to each point in a three-dimensional space, such as a crystal. Vector analysis extends standard algebra by addressing the 'heuristic counter-example' that Leibniz had identified: in vector analysis, variables are specified not just by a quantity (as they are in standard algebra) but also by a direction.

[28] Madame Curie, for example, writes of her husband that he had asked the same questions that Galois had when the latter developed Group Theory, although without apparent knowledge until later about Galois's work. "But he was happy to learn its results in the geometric applications to the case of equations of the fifth degree" (15).

Vector analysis is important for the use of symmetry concepts in the physical sciences because it allows one to generalize from two dimensions to three the formalism for describing and manipulating rotations, which constitute an important class of symmetry operations. There had long been a way to add and subtract vectors (through the parallelogram of velocities) just as there had been ways to manipulate rotations in the plane. But handling rotations in three dimensions is vastly more complex than in two.

The mathematical research programme that underlay the initial development of vector analysis has been a progressive one. This programme concerned the theory of hypercomplex numbers, the type of number that generalizes the complex number system comprising both real and imaginary numbers.[29] Although several mathematicians were working on this independently and at about the same time, it was the discovery of the quaternion number system by William Rowan Hamilton (1805-1865) that led to the development of modern vector analysis. Hamilton had already worked on algebraic couples — ordered pairs of numbers that represent complex numbers — and he was interested to see whether a formalism based on ordered *triples* could extend the complex number system. He failed in that task, but the failure was due not to a personal limitation but to an inherent mathematical difficulty. In the end "he had a flash of inspiration: His difficulty would vanish if he used quadruples instead of triples and if he abandoned the commutative law for multiplication" (Boyer 583). He had discovered quaternions:

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[29] For our purposes, the important point about the history of this mathematical research programme lies not in the detail about these number systems but in the fact that the programme was driven by purely mathematical concerns.

ordered quadruplets of numbers for which a consistent set of mathematical operations could be defined.

This was a progressive problemshift: if we consider Hamilton's programme on hypercomplex numbers in a Lakatosian framework (such as the one set out in *Proofs and Refutations*), we would see how the concept of number had been progressively expanded to embrace ideas of greater and greater generality — moving from real numbers, to complex numbers, to quaternions, and then beyond. Each challenge to the conceptual scheme (each heuristic counterexample) would have forced us to abandon some restrictive property — such as commutativity, to accommodate quaternions, or associativity, for higher algebras, and so on. Histories, such Kleiner's *A History of Abstract Algebra* or Boyer's *A History of Mathematics*, trace that sequence.

To see how much this mathematical research programme could have driven scientific research programmes, we need a physical interpretation of its mathematical expressions. Hamilton himself provided such an interpretation, one in terms of three-dimensional space in which vectors representing physical quantities could be embedded. Although the practical utility of his particular interpretation can only be evaluated *a posteriori*, we can understand why Hamilton posited it. He would have been aware that complex numbers had been represented geometrically in the plane with the two axes corresponding to the real and imaginary components of those numbers.[30] He had also already worked out an algebra for complex numbers considered as ordered real-number

[30] This two-dimensional framework for representing complex numbers is often referred to as an Argand Diagram.

pairs and devised a rule for multiplication of those couples that can be interpreted as a rotation in the plane; in other words, he provided an algebraic interpretation of the symmetry operation of rotation. So it was natural that he try to extend that two-dimensional interpretation of complex numbers to a three-dimensional interpretation of quaternions, since quaternions were the next most general number system that could form a consistent algebra. Specifically, Hamilton posited that a quaternion q, which is an ordered quadruplet (w,x,y,z) of real numbers, corresponded to a vector in three dimensions

$$q = w + x.\mathbf{i} + y.\mathbf{j} + z.\mathbf{k}$$

where **i**, **j**, and **k** are unit vectors in mutually perpendicular directions, subject to the following rules of his algebra:

$$\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}_2 = -1$$

and

i.j = k ; j.k = i ; k.i = j but **j.i = -k ; k.j = -j ; i.k = - j**

Multiplication of quaternions was to be interpreted as a rotation in three-dimensional space (Altmann 41-68).[31]

The mathematical research programme that underlay the initial development of vector analysis, which concerned hypercomplex numbers, did not however drive the further development of the vector analysis used in scientific research programmes. The first vector analysis emerging from that research, Hamilton's, was not developed until 1843, well after the formative stages of the symmetry concept within crystallography in the period 1815-1830. Even after that, his vector analysis turned out to be impractical. There were two main reasons for that: it did not provide the correct answers for calculations of rotation in three dimensions[32] and its vector multiplication[33] did not have a natural interpretation.

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[31] Hamilton, as a Kantian with a Pythagorean commitment to the significance of numbers, would have had no difficulty in claiming that number theory governs geometrical relationships in physical space.

[32] A useable vector analysis would permit one to calculate quite generally what axis and angle of rotation would be equivalent to an initial rotation about a given axis through a certain angle followed by a subsequent rotation about a different axis and through another angle. Hamilton's analysis gives the wrong answer: "the angle of rotation is double the angle which appears in the quaternion" (Altmann 57).

On the contrary though, scientific research programs did drive the further development of vector analysis. They did so by demanding a formalism that was responsive to their emerging inferential needs. The developments were driven not, as it were, by the producers of those vectorial systems (mathematicians) but by their consumers (principally physicists). By the 1870s, "physical science (above all electricity) [had] developed in such a way that the need for a vectorial system increased" (Crowe 251) — but at the same time the deficiencies in the existing formalisms had become apparent. In particular, James Clerk Maxwell (1831-1879) had recognized the importance to electricity and magnetism of a vectorial system with appropriate forms of vector multiplication. Although Maxwell's interest had naturally been aroused by the quaternion system, he was well aware of its limitations, made little use of it, and made his criticisms

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[33] Multiplication has important applications: in crystallography — for calculating rotations and for relating planes, such as crystal faces, to lattice points; in electricity and magnetism, whose symmetries Curie explored with tools developed in crystallography; and in the physical sciences more generally. As Crowe sets out in his history, what we now regard as vector multiplication can be identified with part of Hamilton's quaternion product and with the 'inner' and 'outer' products of Grassmann's vector formalism, the other predominant one of that time (248). Although both Hamilton's and Grassmann's formalisms had elements that could have morphed into our modern concept of vector multiplication (actually comprising two forms: the dot product and the cross product) neither formalism was or is wholly satisfactory, as they contain mathematical elements that are either not equivalent to what we want or even to anything at all (248).

known. His *Treatise on Electricity and Magnetism* passed the conceptual challenge on to two other physicists — the American, Josiah Willard Gibbs (1839-1903) and the Englishman, Oliver Heaviside (1850-1925). Working independently, but coming to equivalent conclusions, they developed the modern system of vector analysis. Although many of the primary results of vector analysis were established by 1880, an ‘Algebra War’ broke out in 1890 and lasted about four years. This ‘war’ was a vehement yet important conceptual debate, mostly conducted between physicists, in which quaternion systems of vector analysis were pitted against the vector analyses that had been developed by Gibbs and Heaviside. Some participants argued that the quaternion systems were “uniquely adapted to Euclidean space” and “natural,” while others argued that the Gibbs-Heaviside system was more streamlined and that it harmonized better with Cartesian coordinates. The Gibbs-Heaviside system is the one currently used in the physical sciences.

Conclusion on this Potential Objection

It is unlikely that any of the mathematical research programmes of the nineteenth century that were most obviously relevant to symmetry alone drove the development of that concept as used in science. In Solid Geometry we have a prefiguration of the modern concept of symmetry in the definition of a solid angle -- but no evidence of a mechanism by which that had any influence on developments in science. In Abstract Algebra we now have the tools to classify crystallography’s conceptual breakthroughs as ‘applications’ of Group Theory -- but this ascription can only be made retroactively since these applications preceded the theoretical framework. And in Vector Analysis we have an extremely useful formalism for incorporating symmetry operations — but one that also arrived too late to shape concepts that emerged in science.

Group Theory and mathematical crystallography had developed quite separately for most of the century, the former unaware of potential application and the latter developing applications in a material context well in advance of any formalization. The two research programs, the applied mathematics of symmetry relevant to crystallography and the pure mathematics of Group Theory, did not interact in any significant way until 1870, when Leonhard Sohncke (1842-1897), a German mathematician, brought them together. He was familiar with Bravais's work but then discovered the 1830 work of Hessel, who had independently discovered the 14 lattices, and the 1869 work of Jordan, who had independently worked on point groups. Hessel and Jordan had both published in obscure journals. Sohncke also added his own work, which included an analysis of two more transformations in three dimensions: the combinations of rotation with translation (the screw axis) and of reflection with rotation (the glide plane).[34] Ever since the union of crystallographic symmetry research with Group Theory it has been possible to assess past contributions to crystallography by using common group theory nomenclature and concepts. Scholz, for example, undertakes a rational reconstruction of the German dynamist contributions in such terms in order to explore the influence of dynamist philosophy on Weiss's research program and the classifications of axial symmetries he

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[34] Combinations are only of interest when they concern two operations that are not separately symmetry-preserving but in combination are such. Since Sohncke's time, the remaining combinations have been analyzed: rotation-reflection and rotation-inversion.

obtained. From a group-theoretic point of view, he sees that Haüy's 18 'primitive forms' are highly redundant because they can be characterized by only eight finite orthogonal groups; that Frankenheim worked out "a complete enumeration of those finite orthogonal groups which arise as point symmetries in crystallography," and that "Hessel derived a complete list of finite point symmetry systems in space, i.e., an implicit but clear representation of all finite orthogonal groups in Euclidean space" ("Rise" 117, 119). As Scholz is at pains to stress, rational reconstruction of historical contributions in no way suggests that the language or concepts used in the era under study were the same as those used now; rational reconstruction is purely an aid to assessment and comparison. "Of course," he says regarding his reconstruction of Frankenheim's contribution, "it was impossible for Frankenheim to use an explicit group concept in the algebraic sense. That was, as is well known, not even formed in algebra itself" ("Rise" 117).

4.6 Further Developments: Physical Symmetry

Physical symmetries, like algebraic ones, are properties that remain unchanged after a transformation, but unlike the algebraic ones considered earlier, need not be restricted to spatial properties like shape. Physical properties, including non-spatial ones, are characterized by magnitudes — single numbers for 'scalar' properties like temperature, triplets of numbers for vector properties like force, and larger groups of numbers for more complex properties like elasticity. Where the transformations are the usual spatial ones (translations, reflections, rotations, etc.), the physical symmetries of a system can help describe a field theory of the physical phenomena in question; that is, they can help describe, but not prescribe, any physical theory that purports to explain the phenomena in terms of physical quantities that have a magnitude at each point in the space.

The historical situation of crystallography and of disciplines related to it helps us understand how the concept of symmetry adapted to meet those new inferential needs. What had helped maintain the progressiveness of the crystallographic research programme was the fruitful synthesis of the French and German crystallographic traditions; the recognition of the need to relate external factors to internal structures was inherited from the French molecularists, while the mathematized algebraic conception of symmetry was inherited from the German dynamists. The particular feature of this synthesis that greatly aided its progressiveness was its representation of internal structure abstractly. This made it possible to avoid commitment to any particular conception of internal structure other than its symmetry. One could make certain symmetry inferences without having to accept an account of the physical constitution of a crystal that was based on the 'molecules' of the French school, the forces of the German school, the atoms of the chemists, or even the unit cells of modern crystallography. Since no empirically adequate theory of any of these effects was available until the twentieth century, it was a clear advantage that neither the lack of agreement on theory nor even the lack of any theory whatsoever would block progress. Nevertheless, research on crystal properties other than external form revealed that, like external form, they also exhibited symmetries. The refraction of light, the conduction of heat and electricity, elasticity, and the generation of electric potentials through heat and pressure were among the phenomena whose symmetries physicists and crystallographers sought to interrelate.

Problem Situation

The problem situation then was to discover how the various physical symmetries are related, even if it was premature to speculate about the mechanisms giving rise to the physical phenomena themselves. Knowing the symmetries of one set of properties may facilitate material inferences about another. This would be very useful for several reasons. First, some physical properties can be measured more easily and more precisely than the traditional ones like cleavage planes, interfacial angles, and crystallographic axes and it would be useful to use them as proxies. Even at the time of Haüy, the British scientist David Brewster had "believed it was much more difficult to gain knowledge of the primitive form by cleavage and calculation than it was to test a crystal for double refraction" (Burke 144). (In time he became confident enough in his optical techniques to challenge some of Haüy's assignments of minerals to crystal classes.) Second, one could use specimens that were crystal only in the sense that they possessed crystalline structure (i.e., having some kind of organized Internal form) even if they were not crystal in the sense of being a shape defined by plane-face boundaries (i.e., having the right sort of external form). Good specimens of the latter are hard to obtain and often have to be grown in controlled conditions to achieve the right degree of perfection. As Walker pointed out in 1914:

> The physical properties in crystals vary with the direction in the crystal but any individual crystal will be found to present the same degree of symmetry from a physical point of view which it presents when geometrically considered. As a result of this remarkable correspondence

> between the physical and geometrical symmetry it is frequently possible by a physical examination of a fragment of a crystal, which does not show any crystal surface, to indicate the system to which it belongs. (41)

Third, it would help to unify the empirical models of the various physical phenomena by reducing the number of independent parameters needed to specify them. Further empirical work was done on this and by mid century Henri Hureau de Sénarmont found many coincidences in symmetric crystals of the crystallographic axes and those of thermal conductivity, electrical conductivity, and optical elasticity (Katzir, *Piezoelectricity* 84), although others found some anomalies. Several problemshifts occurred.

Problemshifts

The basic problemshift was away from the primacy of crystalline form and towards a plurality of interrelated physical symmetries. Katzir attributes this to Franz Neumann, whose "important innovation was the replacement of the crystalline form by symmetry as the organizing principle of the physical study of crystals" ("Physics" 48). This was clearly a progressive move: Katzir notes how various researchers used symmetry considerations phenomenologically (i.e., without recourse to any specific theory of matter) to reduce the number of free parameters in empirical models of physical phenomena and to account for previously anomalous effects. Those efforts include Neumann's own study on elastic behavior in crystals (47) and Voigt's deduction of the piezoelectric coefficients 52).

Curie introduced another important problemshift, which was to use symmetry to make inferences concerning the relationship between physical magnitudes in any medium, crystal or otherwise, and even between theoretical entities like electric and magnetic fields. This was also a progressive move and Curie himself was thereby able to account for certain electric and magnetic phenomena on the basis of symmetry alone (Katzir, "Physics" 56).

A third problemshift, also formally introduced by Curie, concerns the focus on asymmetry rather than symmetry. This seems more like a heuristic principle than a matter of logic. Curie expressed it this way in the second rule of his principle:

> *When certain effects show a certain asymmetry, this asymmetry must be found in the causes which gave rise to them.* (Curie 20)

Unlike the other relationships of physical symmetry, the comparison here is not so much between physical magnitudes as between 'effects' (phenomena, observed to be asymmetric) and their 'causes' (models, including their initial conditions, structures, and laws). Since models that are symmetric in all respects must predict (via deductive logic) outcomes that are symmetric, the presence of an asymmetric outcome is part of a creative process that disqualifies all symmetric models.

5. CONCLUSION

I now review what has been accomplished in this historical epistemology of symmetry and suggest follow-on research that will push the understanding of symmetry inference further.

5.1 The Quest: Symmetry Warrants

I began with a quest. The concept of symmetry, as well as the inferences based on it, has been deeply puzzling. What was it about the concept of symmetry, I asked in Chapter 1, that led to the astonishingly successful use of symmetry inference in the physical sciences? Some thought experiments, like those of Archimedes, seemed capable of generating a whole corpus of scientific results *a priori.* Yet, it must be admitted, other symmetry inferences turned out to be utterly wrong, despite the initial 'obviousness' of their conclusions — the disconfirming observations in these cases being described by contemporary scientists as 'shocks' or 'violations.' For example, in the early nineteenth century, the Danish physicist Ørsted reputedly wasted eight years of research effort because of a firm conviction about the direction in which a magnetic needle would deflect in the presence of an electric current, a conviction based on a symmetry inference. So, two warnings should jump out from just this last example: symmetry inferences may not all be *a priori* after all and the cost of getting them wrong might be high.

To be clear about the questions we might pose concerning symmetry inference, I argued in Chapter 2 that we need to seek *material* warrants, not logical ones, and distinguished among three possible warrants for which we may be searching. The projectable warrant underwrites, as it were, the continued use of a symmetry concept for inferences within a given research program, i.e., what makes it projectable to instances other the ones originally used in positing that concept. The evolvable warrant underwrites the continued success over time of resorting to some variant or other of the *symmetry* concept specifically, perhaps by modifying an existing symmetry concept inside the field or by importing one as a metaphor from outside. The transferable warrant underwrites the transfer of the patterns of symmetry inference from one field to another.

In the literature, the closest parallel for finding warrants is the analysis of the 'unreasonable effectiveness' of mathematics (to use an expression made famous by the physicist Eugene Wigner). This is because the standard view of symmetry inferences in the physical sciences, mostly implicit and rarely critiqued, is that symmetry is a fundamentally mathematical concept and, therefore, that inferences based on symmetry are warranted because they inherit the certainty of mathematics. The problem with this view is that it does not address *applicability* of any particular variant of the concept of symmetry to a given physical situation. Applicability is neither self-evident nor mathematically provable, and revering effectiveness as a mystery is certainly unhelpful. Since I have argued already that symmetry is a fundamentally material concept, I treated it as a concept that had emerged and developed over time within the sciences. In this view, inferences based on symmetry, which are always fallible, are warranted to the extent that the concept of symmetry has co-adapted with the sciences whose inferential needs it supports. Ian Hacking, with his idea of self-vindication of the laboratory sciences, Bas van Fraassen, with his selectionist account of the success of science, and Steven French, with his adaptationist account of the introduction of group theory, follow the same line of thought, although none has addressed the specific issue I have identified.

In order to best exhibit what a material warrant for symmetry inference would look like, I followed the best-practice examples of closely related historical epistemologies. These generally identify the inferential practices facilitated by a given concept, the ways later forms of a concept derive from earlier ones, and the triggers of conceptual adaptation. In Chapter 3 I argued that certain features of the historical approach of Lakatos were also helpful, particularly in the way it distinguishes between successful and unsuccessful phases of a research program. I chose early nineteenth-century crystallography as the most propitious for exhibiting symmetry warrants because it is generally accepted that symmetry inferences emerged and developed there.

5.2 Key Findings: Inferential Practices and Conceptual Adaptation

The key findings of the case study in Chapter 4 are that material warrants for symmetry inference can be expressed in terms of inferential practices and conceptual adaptation. I was able to track the role of symmetry in inferential practices throughout the study period, to identify the changes in the symmetry concept, and also to associate those changes specifically with selective pressures on research programs to mitigate arbitrariness (such as *ad hoc* assumptions, brute facts, and arbitrary procedures). Therein lies the projectable warrant: the effect of conceptual changes is to make the symmetry concept more projectable, more capable of leading to inferential success without having to be retrofitted to observational data case-by-case.

To show what these projectable warrants look like, it was necessary to delve into the historical details of particular fields, because material inferences depend on content and context, not mere propositional form. I found that there had been a succession of symmetry concepts — each either derived as a modification of an earlier one in the field or introduced as a metaphor from the wider culture — and that the introduction of each variant of symmetry had reduced program arbitrariness and increased projectability. The details are in the text, but in summary I noted the following. Initially, a concept of aesthetic symmetry had been introduced to reduce the myriad brute facts about crystal shape; if crystal shapes could be derived in a non-arbitrary way from a small number of primitive forms having 'fitting' or 'appropriate' proportions, then one would have to accept, as the arbitrary givens, only a small number of aesthetic norms rather than a large number of shapes. But that had still left an unacceptably large degree of theoretical discretion in the choice of primitive forms needed to match observed shapes. A 'molecular' model had then been introduced to minimize that, but it too required choices to be made about the way its molecules had to be stacked to generate the observed shapes. So those choices in turn had to be constrained by geometric symmetry, the assumption that crystal faces with the same geometric shape and similarly situated in the crystal must support identical crystal structures. But once crystal phenomena other than shape began to be studied intensively, especially those with directional properties like optical and electrical phenomena, it became necessary for the molecularists either to study them *ad hoc* or to arbitrarily exclude from study the crystals in which they occur.

That soon became moot when a rival program, using a concept of algebraic symmetry, was able to provide an account.

Another key finding is that the historiographical data does not support rival claims that the scientific concept of symmetry emerged and developed in mathematics and then moved to the physical sciences. (I had already argued on general grounds that symmetry inference was a material inference, so this finding is not unexpected; but it nevertheless further punctures the assumption that warrants are mathematical in nature.) In the case of solid geometry, there is no historiographical record to back up the claim that the definition of symmetry offered by Legendre had any influence on the development of crystallography. In the case of group theory, the development and dissemination of the theory postdated the developments in crystallography. In vector analysis, where the relationship is a little less direct, the formalism did arise in mathematics but failed in application until it was completely reworked by physicists.

The case study has a few shortcomings; these however can be mitigated.

- First, the historical trajectory of the symmetry is contingent. We know that the concept of symmetry emerged in crystallography before 1830 and that it then developed through being successively adjusted to apply to a variety of physical properties. But would we have the same concept if it had first developed in (say) the early work on electromagnetism by Ørsted and others, also around 1830, only later being transferred to crystallography? Would it matter if the concept emerging from that process differed from the one we actually have? Further case investigations should be able to identify the conditions that favored development in one field rather than another and address these questions.

- Second, only half a dozen problemshifts were considered in the case study. Although it was quite clear in each case how the conceptual changes addressed arbitrariness, a more extensive study, covering developments in the latter part of the nineteenth century, would help to strengthen that particular observation.
- Third, the concept of 'mechanism,' which I have used in my description of concept change, is undefined and philosophically problematic. In any subsequent work of this nature, one would need to be more precise about this. Suffice it to say that I am asserting not only that the concept of symmetry changed at certain times and that the change had the effect of reducing arbitrariness, but also that the change is explained by the fact that it was introduced for the sake of that effect. (Lest it be thought that this judgment is an anachronistic artifact of the Lakatosian categories I have used for descriptive and analytical purposes, I have also included historiographical evidence in the case study to the effect that contemporary reviewers themselves compared rival research programs on the basis of the distinction between principled and arbitrary postulates.)

5.3 Further Reflections: Experimental Restraints on the Practice of Theorizing

Adventitious findings and broader reflections provide insights that go beyond the key findings, since the latter mainly focus on how well initial expectations were confirmed. I highlight below some of the more significant insights.

Ontological Restraint

In the period covered by the case study, experimentalists found ways to make significant material inferences with only minimal metaphysical commitment. The first truly scientific study of crystals, Haüy's, the hard core of the research program included a commitment to a particular molecular view of matter. Symmetry concepts were ancillary; they were instruments to reduce the arbitrariness in the shapes of building blocks and in the ways they were stacked. The subsequent theory of Weiss was also inspired by a theory of matter, one comprising inner forces kept in balance. In this case I noted that it was the *symmetry concept* he used that was part of the hard core of his program, not his *metaphysical theory*. It had turned out that the theory had almost no influence on later developments and its specific tenets were neither empirically tested nor defended. The algebraic symmetry that Weiss introduced though had major, long-lasting ramifications. It unleashed a large program of mathematization as crystallographers found new ways to organize their laboratory findings on the physical properties of crystals. After the intense period of mathematization, the notion of 'inner structure' was re-introduced, not as requiring molecules or forces, but as the bare-bones postulate of the crystal lattice — in effect no more than internal symmetry. As a result, by mid-century certain inferences could be made with very little theory at all. This made it possible for a later generation of French molecularists and German polar theorists to collaborate fruitfully without being diverted by debates over the 'deeper' meaning of their work.

Beyond the period covered by the case study, crystallographers continued in the same vein, making progress in the absence of physical theories about light and electricity. For example, in 1848, Pasteur discovered that solutions of certain substances rotate the plane of light's polarization in a way that depends on that asymmetry of the crystal form of that substance; although he himself linked the asymmetry of the crystals he used to the asymmetry of their molecules, his belief in molecules played no essential role in that inference. Around 1880, Pierre Curie and his brother Jacques discovered piezoelectricity (the production of electricity in crystals by pressure) and that phenomenon was explored extensively over the following 15 years. As a result, researchers discovered the types of crystal symmetry necessary for the possibility of piezoelectricity, those necessary for pyroelectricity (the production of electricity in crystals by heat), and the relation between the two types — all without theories of matter or electromagnetism.

The upshot is that by using symmetry considerations experimental scientists can often avoid having to take sides in a theoretical debate. They can still make the conceptual adaptations needed to facilitate their work, make scientific progress in their field, and, moreover, find common ground with other scientific communities.

The Dichotomy of Principled and Arbitrary Choice

In the period of the case study, what emerges as the separator between rival research programs is the distinction between principled and arbitrary choices of theoretical postulates. Arbitrary choices can threaten the integrity of research programs in at least two ways. The first is that if choices are left up to individual experimenters there will be no accounting for taste and little basis for dialogue or independent replication. The second is that researchers can vitiate experimental testing by making arbitrary choices of assumptions or parameters in order to retrofit their theories to the data. Symmetry concepts offer ways to minimize those dangers.

I discern, both within and beyond the case study, several ways in which symmetry can respond to issues of arbitrariness. One response is to *privilege* one, or a few, among the many conceivable options, the way Haüy did using an aesthetic symmetry. Such a concept of symmetry is inferential only insofar as aesthetics is regarded as having normative force, that is, insofar as we agree that certain numerical proportions are fitting, appropriate, or natural. (Despite being clearly problematic, such criteria are major factors today in the choice between rival theories.) A second response is to *equivalence* the options, the way Weiss did by deeming certain points-of-view of a crystal to be equivalent. A third response is to *idealize* a physical situation -- the way theoretical scientists sometimes do, when using an approximate or abstract symmetry. In these cases, certain physical situations known to be different are regarded as equivalent in an abstract sense (the neutron and the proton are both nucleons, for example) or their known differences regarded as irrelevant for the purpose at hand.

Material Warrants

The case study shows directly how the projectable warrant can be established; it also indicates how the other inferential warrants could be grounded in a similar way.

The evolvable warrant, for example, is likely to be revealed in a historical study of late nineteenth-century crystallography. In the early decades of the nineteenth century, symmetry concepts were part of the protective belt where they were used to defend hard core commitments. Hard core commitments, protective belt maneuvers, and anomalies were *disparate* kinds of things; for example, in the program of Haüy, they were molecular forms, symmetries, and angles respectively. By mid-century though, the positive heuristic that had developed in the then-dominant German crystallographic tradition had changed. Hard core commitments, protective belt maneuvers, and anomalies were by then *kindred*; specifically, they were all symmetries. That set up a virtuous feedback loop in which 'anomalies' were likely to be regarded less as flaws fatal to the whole program and more as data that could trigger the further evolution of 'higher' symmetries. This, I speculate, is the reason that when experimentalists needed to make adjustments to their research programs they immediately reached out for another *symmetry* concept. Researchers in the second half of the century learned how to determine the symmetries of physical properties other than shape (such as optical, thermal, electrical, and mechanical properties) and, in a self-vindicating way, turned those new symmetries into the *data* of the program, properties that had never been observed before because nobody had defined them or thought to look for them.

5.4 Further Research: Self-Vindication and its Limits

It behooves us to understand the nature of symmetry inference as well as we can, not only because the philosophical payoffs could be significant, but because the symmetry-based investments and research efforts in the sciences are very substantial. For philosophy, further research on symmetry inference would provide insights into theory choice, into the use of historical epistemology for understanding and grounding forms of inference, and into restraining the practice of theorizing. For the sciences to which symmetry inference has recently been introduced from another domain, further research would reveal whether we need to establish its symmetry warrants from, as it were, the ground up (the way it was done here for crystallography) or whether we need to show that existing symmetry warrants transfer from the source domain.

It is in the field of physics where we have the most vivid image of what is at stake: not Ørsted's experimental setup but the Large Hadron Collider, the most powerful particle collider in the world. It was built at a cost of about $10 billion and operates on an annual budget of around $1 billion. That alone makes it important to stand back from the specific theories it will test, all involving symmetry in one form or another, and to examine their warrants.

There are two areas where the work of this thesis specifically could be profitably extended: evolvable warrants and transferable warrants.

Evolvable Warrants

The first would cover crystallography in the second half of the nineteenth century since, as I mentioned above, that era provides the best case material for a study of the evolvable warrant.

When Curie stated in 1894 that there was "interest in introducing into the study of physical phenomena the symmetry arguments familiar to crystallographers," he must have been referring to physical phenomena occurring *outside* crystals. This is because he was by then already able to look back on many decades of research into physical phenomena *inside* crystals.

This research extension would aim to determine whether a coherent material account can be given for the evolvable warrant in terms of conceptual adaptation and the self-vindicating laboratory practices that become possible once symmetry itself becomes the prime focus of study. This suggests that we may be able to read the famous Curie Principle, *When certain causes produce certain effects, the symmetry elements of the causes must be found in their effects. When certain effects show a certain asymmetry, this asymmetry must be found in the causes which give rise to them*

as a codification of the developing heuristic rather than as either a tautology or a re-statement of the principle of causation (as some have suggested, including Curie himself through his choice of terms ‘cause’ and ‘effect’).

Transferable Warrants

The second research extension would cover several sciences in the twentieth century where different routes of transfer seem possible. This extension would aim to determine whether a coherent material account can be given for the transferable warrant. I hypothesize, for example, that symmetry reasoning was indeed transferred from crystallography to stereochemistry and that the warrant for that relied on a common laboratory culture, the common use of three-dimensional spatial representations, and the historical link between crystallography and chemistry (Pasteur, for example). By contrast, I hypothesize that while the same reasoning was transferred to particle physics, that transfer was accomplished only via the mathematics of group theory and not through any shared practices. If so, it follows that any warrant for the abstract symmetry inferences in particle physics would have to be grounded in other ways.

One of the tough philosophical challenges that Curie left us at the end of the nineteenth century is to understand the transferable warrant — and whether any such warrant can apply to abstract symmetries that are neither spatial nor analogous to any properties studied in the laboratory sciences.

…

Curie was right to think that symmetry arguments are special and warranted, that they arose in crystallography, and that they can be used in physical sciences. Showing the conditions under which they are warranted though requires detailed work — not just mathematical, but historical.

REFERENCES

CP Collected Papers of Charles Peirce

DK Diels–Kranz (DK) numbering is the standard system for referencing the works of the pre-Socratic philosophers

Altmann, Simon L. *Icons and Symmetries.* Clarendon, 1992.

Archimedes. “On the Equilibrium of Planes,” Book I. *The Works of Archimedes*, translated by T. L. Heath, Cambridge UP, 1897, pp. 189-202.

Aristotle. “De Caelo.” Trans. J. L Stocks. *The Basic Works of Aristotle*. Edited by Richard McKeon, Modern Library, 2001, pp. 398-466.

Atkins, Peter and Julio de Paula. *Physical Chemistry: Thermodynamics, Structure, and Change.* Tenth ed. , W.H. Freeman.

Benninga, H. *A History of Lactic Acid Making: A Chapter in the History of Biotechnology.* Kluwer, 1990.

Bensaude-Vincent, Bernadette and Isabelle Stengers. *A History of Chemistry.* Trans. Deborah van Dam. Harvard UP, 1996.

Borchardt-Ott, Walter. *Crystallography: An Introduction. Trans. Robert O. Gould. 3rd ed. Springer, 2011.*

Boyer, Carl B. and Uta C. Merzbach. *A History of Mathematics.* Second Edition. Wiley, 1991.

Brading, Katherine and Elena Castellani. “Introduction.” *Symmetries in Physics: Philosophical Reflections*, edited by Katherine Brading and Elena Castellani, Cambridge UP, 2003, pp. 1-18.

Brigandt, Ingo. “Scientific Reasoning is Material Inference: Combining Confirmation, Discovery, and Explanation.” *International Studies in the Philosophy of Science,* vol. 24, no. 1, 2010, pp. 31-43.

Brochant de Villiers, [André-Jean-François-Marie], translator. “*Dissertatio de Indagando formarum crystallinarum Caractere geometrico principali*, ou Mémoire sur la détermination du caractère géométrique principal des formes cristallines.” *Journal des Mines*, Vol. 19, 1811, pp. 349-391; 401-444.

Brooke, H.J. “Observations on a Memoir by the Abbé Haüy on the Measurement of the Angles of Crystals.” *Annals of Philosophy*, vol.14, 1819, pp. 453-456.

Buée, A.-Q. “Outlines of the Mineralogical Systems of Romé de l’Isle and the Abbé Haüy: with Observations.” *Nicholson’s Journal,* Vol. 9, 1804, pp. 26-39.

Burke, John. G *Origins of the Science of Crystals.* University of California P, 1966.

Burks, Arthur W. “Peirce’s Theory of Abduction.” *Phil. Science*, vol. 13, no. 4, 1946, pp. 301-06.

Castellani, Elena. “On the Meaning of Symmetry Breaking.” *Symmetries in Physics: Philosophical Reflections*, edited by Katherine Brading and Elena Castellani, Cambridge UP, 2003, pp. 321-34.

Crowe, Michael J. *A History of Vector Analysis: The Evolution of the Idea of a Vectorial System*. 1967. Dover, 1985.

Curie, Marie. *Pierre Curie*. 1923. Translated by Charlotte and Vernon Kellogg, Dover Publications, 2012.

Curie, P. “On the Symmetry in Physical Phenomena, Symmetry of an Electric Field and of a Magnetic Field.” Originally published in French in *Journal de physique*, 3rd series, Vol. 3, 1894, pp. 393-415. Translated by J. Rosen and P. Copié. *Symmetry in Physics: Selected Reprints*, edited by Joe Rosen, American Association of Physics Teachers, 1982, pp. 17-25.

Cuvier, G., editor. “Rapport historique sur le progrès des sciences naturelles depuis 1789 et sur leur état actuel.” *Institut de France*. 1810, p.17.

Daston, Lorraine and Peter Galison. *Objectivity*. Zone Books, 2007.

Dewey, John. *Logic: The Theory of Inquiry*. Holt, 1938.

- - -. “Propositions, Warranted Assertability, and Truth.” *The Journal of Philosophy*, Vol. 38, No. 7, 1941, pp. 169-186.

Du Sautoy, Marcus. *Symmetry: A Journey through the Patterns of Nature.* Harper, 2008.

Emerton, Norma E. *The Scientific Representation of Form*. Cornell History of Science Series. Cornell UP, 1984.

Feest, Uljana and Thomas Sturm. “What (Good) is Historical Epistemology? Editors’ Introduction.“ *Erkenntnis*, Vol. 75, No. 3, 2011, pp. 285-302. doi 10.1007/s10670-011-9345-4.

French, Steven. “The Reasonable Effectiveness of Mathematics: Partial Structures and the Application of Group Theory to Physics.” *Synthese*, Vol. 125, No. 1/2, Festschrift in Honor of Newton C. A. Da Costa on the Occasion of His Seventieth Birthday, Oct-Nov. 2000, pp. 103-20.

Geison, Gerald L. “Louis Pasteur.” *Dictionary of Scientific Biography*, edited by Charles Coulston Gillespie, Vol. 10, American Council of Learned Societies, 1981.

- - -. *The Private Science of Louis Pasteur.* Princeton UP, 1995.

Hacking, Ian. *The Emergence of Probability: A Philosophical Study of Early Ideas about Probability, Induction and Statistical Inference*. Cambridge UP, 1975.

- - -. *Representing and Intervening*. Cambridge UP, 1983.

- - -. “The Self-Vindication of the Laboratory Sciences.” *Science as Practice and Culture*, edited by Andrew Pickering, U Chicago P, 1992, pp. 29-64.

“Haüy, René-Just”. *Dictionary of Scientific Biography, e*ditor-in-chief, Charles C. Gillespie. Vol. 6, Charles Scribner’s Sons, 1970-80, pp. 178-83.

Haüy, René-Just. *Traité de minéralogie*, 5 vols, Louis, 1801.

Heath, T. L. *The Works of Archimedes*. Cambridge UP, 1897.

“Hessel, Johann Friedrich Christian.” *Dictionary of Scientific Biography, e*ditor-in-chief, Charles C. Gillespie. Vol. 6, Charles Scribner’s Sons, 1970-80, pp. 358-59.

Hon, Giora and Bernard R. Goldstein. “Legendre’s Revolution (1784): The Definition of Symmetry in Solid Geometry.” *Archive for the History of the Exact Sciences,* Vol. 59, No. 2, 2005, pp. 107-55.

- - -. *From* Summetria *to Symmetry: The Making of a Revolutionary Concept*. Springer, 2008.

- - -. "The Double Face of Symmetry: A Conceptual History." *Nova Acta Leopoldina,* Nationale Akademie der Wissenschaften, NF Nr. 412, 2016, pp. 45-73. Downloaded 10 Feb 2019, leopoldina.org.

Katzir, Shaul. "The Emergence of the Principle of Symmetry in Physics." *Historical Studies in the Physical and Biological Sciences,* Vol. 35, No. 1, 2004, pp. 35-65.

- - -.. *The Beginnings of Piezoelectricity: A Study in Mundane Physics*. *Boston Studies in the Philosophy of Science*, general editors, Robert S. Cohen *et. al*., Vol. 246. Springer, 2006.

Kepler, Johannes. *The Six-Cornered Snowflake*. 1594. Trans. Jacques Bromberg. Paul Dry Books, 2010.

Kleiner, Israel. *A History of Abstract Algebra*, Birkhäuser, 2007.

Kubbinga, Henk. "Crystallography from Haüy to Laue: Controversies on the Molecular and Atomistic Nature of Solids." *Acta Cryst.* A68, 3–29, 2012, pp. 3-29, doi:10.1107/S0108767311030315

Lakatos, Imre. *Proofs and Refutations*. Cambridge UP, 1976.

- - -. "The Methodology of Scientific Research Programmes." *Philosophical Papers,* Vol. 1. Cambridge UP, 1978.

Mach, Ernst. *The Science of Mechanics: A Critical and Historical Account of its Development*, 1893, translated by Thomas J. McCormack, Open Court, 1919.

Martin, Christopher A. "On Continuous Symmetries and the Foundations of Modern Physics." *Symmetries in Physics: Philosophical Reflections*, edited by Katherine Brading and Elena Castellani, Cambridge UP, 2003, pp. 29-60.

Norton, John D. "A Material Dissolution of the Problem of Induction." *Synthese*, Vol. 191, 2014, pp. 671-90.

Pasteur, Louis. "Leçons de Chimie profesées en 1860." Presented to the Chemical Society of Paris, January 20 and February 3, 1860. Reprinted as "Researches on the Molecular Dissymmetry of Natural Organic Products," translated by W.S.W. Ruschenberger, *American Journal of Pharmacy*, January, 1862, pp. 1-32.

Peirce, Charles Sanders. *The Collected Papers of Charles Sanders Peirce,* Vol. 1-6. Edited by Charles Hartshorne and Paul Weiss, Harvard UP, 1931-35.

Phillips, F. C. *An Introduction to Crystallography*, 4th ed. Wiley, 1971.

Pickering, Andrew. "From Science as Knowledge to Science as Practice." *Science as Practice and Culture*, edited by Andrew Pickering, U Chicago P, 1992, pp. 1-26.

Plato. "Timaeus*"*. 17a-92c. Translated by Peter Kalkavage. *Plato:Timaeus,* 2nd. ed., Focus-Hackett, 2016.

Popper, Karl. *Objective Knowledge*. Oxford UP, 1972.

Putnam, Hilary. *Mathematics, Matter and Method*. Volume 1. Cambridge UP, 1975.

Renn, Jürgen. "The Relativity Revolution from the Perspective of Historical Epistemology." *Isis*, Vol. 95, No. 4, 2004, pp. 640-48.

"Review of M. Haüy's *Traité de Mineralogie*." *Edinburgh Review,* Vol. 3, 1803, pp.44-46.

Rheinberger, Hans-Jörg. *On Historicizing Epistemology.* Translated by David Fernbach. Stanford UP, 2010.

Rogers, Austin F. "A Mathematical Study of Crystal Symmetry." *Proc. of the American Academy of Arts and Sciences,* Vol. 61, No. 7 ,1926, pp. 161-203.

Rosen, Joe. *Symmetry Rules: How Science and Nature are Founded on Symmetry*. Springer, 2010.

Rosen, Joe, editor. *Symmetry in Physics: Selected Reprints.* American Association of Physics Teachers, 1982.

Sands, Donald E. *Introduction to Crystallography: An Introduction.* 1969 and 1975. Dover, 1993.

Selzer, Michael. *Symmetry Fallacies*. KeepAheadPress, 2018.

Scholz, Erhard. "The Rise of Symmetry Concepts in the Atomistic and Dynamist Schools of Crystallography, 1815-1830." *Revue d'histoire des sciences*, Vol. 42, No. 1/2, *La mathématisation* 1780-1830, 1989, pp. 109-22.

- - - ."The Influence of Justus Grassmann's Crystallographic Works on Hermann Grassmann." *Hermann Günther Graßmann (1809-1877): Visionary*

Mathematician, Scientist and Neohumanist Scholar, edited by G. Schubring, Kluwer Academic Publications, 1996, pp. 37-45.

Schuh, Curtis P. *Mineralogy & Crystallography: On the History of these Sciences from Beginnings through 1919*. Unpublished notes. Tucson, 2007, www.ia800702.us.archive.org.

Schwichtenberg, Jakob. *Physics from Symmetry*. Springer, 2015.

Steiner, Mark. *The Applicability of Mathematics as a Philosophical Problem.* Harvard UP, 1998.

Sternberg, Shlomo. *Group Theory and Physics*. Cambridge UP, 1994.

Stewart, Ian. *Why Beauty is Truth: A History of Symmetry*. Basic Books, 2007.

Szwacki, Nevill Gonzalez and Teresa Szwacka. *Basic Elements of Crystallography*. Pan Stanford, 2010.

Van Fraassen, Bas C. *The Scientific Image.* Clarendon, 1980.

- - -. *Laws and Symmetries*, Clarendon, 1989.

Wadsworth, M. Edward. *Crystallography: An Elementary Manual for the Laboratory.* John Joseph McVey, 1909.

Walker, T.L. *Crystallography: An Outline of the Geometrical Properties of Crystals.* McGraw-Hill, 1914.

Weiss, Christian Samuel. *De Indaganda formarum crystallinarum charactere geometrica principale* … Tauchnitz, 1809. Trans. Kubbinga 16.

Weyl, Hermann. *Symmetry*, Princeton UP, 1952.

Wigner, Eugene P. "The Unreasonable Effectiveness of Mathematics in the Natural Sciences." 1959. *Symmetries and Reflections*, Indiana UP, 1967, pp. 222-37. Richard Courant Lecture in Mathematical Sciences delivered at New York University, 11 May 1959 and originally published in *Communications in Pure and Applied Mathematics,* Vol. 13, No. 1, 1960.

Wilson, Mark. *Wandering Significance*. Clarendon Press, 2006.

Wray, K. Brad. "A Selectionist Explanation for the Success and Failures Science." *Erkenntnis*, Vol. 67, No. 1, 2007, pp. 81-89.

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