

PHILOSOPHICAL AND HISTORICAL INTRODUCTION

HINNE HETTEMA

Department of Philosophy, The University of Auckland
Auckland, New Zealand

The papers collected in this volume all deal with the genesis of the modern theory of the atom, molecules and the chemical bond. The genesis of quantum mechanics is studied extensively in the philosophy of modern science, but the study of atomic theory generally, and particularly the evolution of chemical explanation using quantum mechanics is not very well represented in these studies.

Quantum chemistry is one of the fields in which the geographical focus almost completely moved continents at the beginning of the thirties. Before roughly 1930, most of the work in this area was done on the European continent — notably Germany — and published in German journals. In the time span of a very few years, quantum chemistry became an American discipline, with publications mainly in English. The present translations provide some evidence of just how big a change in perspective this was — for many contemporary readers, the line of argument in many papers might appear very unfamiliar. The aim of this introduction is to document this shift¹ and summarise some recent material. We will mainly discuss the viewpoint of the early continental quantum chemistry community, dwelling on the cultural climate of Weimar Germany and the context in which the papers collected in this volume were written. The American point of view is better documented at present and moreover falls outside the scope of the present collection.

¹Part of this has already been done, notably in the recent book by Mary Jo Nye on the genesis of theoretical chemistry from its background in “chemical philosophy” (Nye 1993) and the article by Gavroglu and Simoes (1994). These two references provide a lot of material which is complementary to the present discussion, especially for the development of the early theories. Nye discusses the interaction between theories and scientific communities, the scientific “style” of the communities and the emerging theories in large detail and it is difficult to really add to her discussion. Gavroglu and Simoes discuss the emergence of quantum chemistry mainly from the American point of view. In his recent biography of Fritz London Gavroglu also provides a lot of background material (Gavroglu 1995). The autobiographies of Hund (Hund 1974) and Mulliken (Mulliken 1968) also provide a part of the background. More general information on the birth of quantum mechanics is found in the biographies of Bohr (Pais 1991) and Heisenberg (Cassidy 1992). The paper published by Max Dresden in a recent festschrift for the Dean of Science from the University of Groningen (Van retort tot Rector, RUG 12 juni 1992) draws attention to the same shift of style (Dresden 1992). The article by Assmus (Assmus 1992) provides additional background material on the molecular tradition in the old quantum theory, which is not the subject of the present discussion.

This chapter will present an overview of these studies to introduce the reader to the main argument and provide the historical background to the papers presented in this book: it is not aimed at providing a radically different perspective.

The point that emerges from the historical evidence is this: the “American” quantum chemistry community was largely and deliberately “pragmatic” in its approach to the emerging quantum chemistry. It consisted mainly of chemists, who worked in an environment in which established barriers between the disciplines were not very strong. The German community, in opposition, consisted mainly of physicists and had a more “theoretical” outlook, which favoured practical applications to a lesser degree. In the German environment, physics and chemistry were more separated. In comparison to the general milieu of Weimar Germany, the early American quantum chemists were very focused on experimental proof and verification.

Therefore, and for the fact that the Nazis rose to power in 1933, attempting to obliterate what they perceived as “Jewish science” and replace it with “Aryan science”, quantum chemistry did not “fit in” very well in the academic milieu in which it originated.

In this introduction, we will elaborate this point. In Section 1 we will give a brief overview of the characterisation of scientific practices. In Section 2, we will outline the structure of scientific practice in Germany, which determined the conditions under which the theory of the chemical bond was developed. This section contains a lot of historical material which, I think, illustrates the context of some debates on the relative role of chemistry and physics in quantum chemistry. We then go on to discuss the field of enquiry of chemistry before and after the birth of the old and the new quantum mechanics.

1. Characterisation of a scientific practice

It is now customary in science studies to characterise scientific “practices” or “disciplines” as the starting point of enquiry. One of the first to introduce the idea of an embedding of knowledge in a social practice was Ludwik Fleck’s *Entstehung und Entwicklung einer wissenschaftliche Tatsache* (“Genesis and development of a scientific fact”) (Fleck 1979), which later heavily influenced Kuhn’s well-known *Structure of Scientific Revolutions* (Kuhn 1970).

The central element of Kuhn’s *Structure* is the “paradigm”, which is an amalgam of core ideas, values, experimental and social practices. A “paradigm” is a complicated concept, of which twenty-one different interpretations have been identified (Masterman 1970) in a close reading of Kuhn’s book.

It is thus not easy to present an exhaustive overview of the “paradigmatic” aspects of a scientific field or practice. In Nye’s study of the development of scientific practice (Nye 1993) in chemistry and physics, she identifies six characteristics of a scientific discipline. Although this list is not exhaustive, we will also use it here. Briefly, the six characteristics are the following:

1. *Genealogy*, “including historical mythology of heroic origins and heroic episodes” (page 19). Genealogy covers the aspects of the continuity of the practice, in terms of intellectual descendency and an established history of the subject. As Nye states, “the authority of continuity is compelling”.
2. *A core literature*. As such we have the books everyone in the field is supposed to have read or be familiar with. These “classics” form a common frame of reference, a common accepted formulation of problems and their solutions, and embody the “standard” science in the sense of Kuhn.
3. *Practices and rituals* that are codified and performed. This aspect covers the “ritual and tacit knowledge” (page 24), participation and organisation of conferences, proceedings, festschrifts and colloquia — in short, all aspects belonging to the social sphere of being part of an intellectual community.
4. *A physical homeland*. As such we mean especially the institutions of the discipline, its laboratories, equipment, and to a certain extent even its (physical) subject matter.
5. *External recognition* of the discipline as a discipline by others.
6. *Shared values and unsolved problems*.

In the following discussion, we will adhere more or less to this characterisation. All of these points, to a certain extent, are a mixture of “social” and “cognitive” aspects.

Quantum chemistry, on every interpretation of a “scientific practice”, was a discipline that was uprooted and replanted around 1930. Some of the evidence in the following section will suggest that quantum chemistry did not flourish too well in its original surroundings, and as a discipline, was much better adapted to its new environment. Particularly, it can be argued that some of the aspects of identity mentioned by Nye were not present in Weimar Germany, but were present in the USA.

2. The academic atmosphere in Germany and the USA

In this section, we will comment on how the general cultural background in the Weimar republic and the USA influenced the relation between chemistry and physics and with it the emergence of quantum chemistry in Germany and its subsequent movement to the United States.²

Some comments are necessary at the start to avoid future misunderstanding. Sometimes quite a lot is made from the fact that Weimar Germany was a country in crisis mood. Especially, the article by Forman (1971) is often interpreted as stating that the physicists in Weimar Germany “caved in” to the outside pressures

²Similarly, in a somewhat different context but in the same vein, Eckert (1996) draws attention to the climate in Germany and contrasts it with other countries. His focus is on theoretical physics. Mehtens (1996) discusses the situation of mathematics in Germany, and draws similar conclusions.

of irrationality, crisis and decay.³ The suggestion is then that the social situation present in Weimar Germany somehow “constructed” quantum mechanics. I do not think this thesis can be maintained. Instead I argue that the outside environment, present in Weimar Germany and the USA, has influenced the embedding and acceptance of quantum chemistry in the wider scientific community in Germany and the USA.

With this out of the way, we can construct the argument.

2.1. The conventionalist argument: Heinrich Hertz’s philosophy of science as an example

At the end of the nineteenth century, German physicists were often engaged, next to physics, in the philosophy of physics. Physics textbooks were often preceded by long introductions dealing with philosophical issues. Especially, Hertz’s introduction to “*The principles of mechanics, presented in a new form*” (Hertz 1956), published after his death in 1894, is still a philosophical classic. Hertz’s view on physics illuminates quite a few of the issues we will encounter later on.

Hertz developed a “picture” theory of scientific propositions. Science, according to him, proceeded by the creation of images, “pictures” of events, and used logical analysis of these pictures to make accurate predictions. These “pictures”, according to Hertz, consisted of three separate components: in the first place, a picture has to be “permissible”, by which Hertz meant it has to agree with our laws of thought. In the second place, they have to be “correct”, which means that they give an accurate representation of the state of affairs. In the third place, they have to be appropriate. The latter condition means that they have to order experience in such a way that our theories are simple and convenient.

What exactly is meant by that? Stated in short, “appropriateness” for Hertz means that it is possible to reformulate our theories with different theoretical terms and principles, while the set of experimental data which is explained by the theory remains the same. In continental science, and especially in Germany, such reformulations were not seen as trivial; in some quarters, they would become the very core of theorising.

Hertz’s view is specific, but in the climate of late nineteenth century Germany by no means peculiar. “Appropriateness” is to a large extent similar (but not identical) to a Kantian “synthetic *a priori*”, which, in the view of the neo-Kantians, is

³Forman, however, discusses mainly the popular writings in physics, such as popular lectures and articles, contributions on the philosophy of physics (not unusual in the German physics environment) and some letters. He does not deal in detail with the content of the scientific theories that emerge from this background. While it is quite conceivable that the outside environment influences the way in which scientists present and communicate their ideas to the wider public and try to attract funding by adhering to the prevailing moods, the notion that the actual content of science is in some way “caused” by the wider environment is much harder to defend. Nevertheless, this seems to be the way in which the “Strong Programme” sociologists reconstruct Forman’s paper. They place Forman in a tradition which “investigate[s] the contingent determinants of belief and reasoning without regard to whether the beliefs are true or the inference rational” [Barnes and Bloor (1982); p. 23].

necessary to make our observations of the physical world at all intelligible. What distinguishes such late nineteenth century ideas from the previous ideas of Kant is the idea that “appropriateness” is not fixed over time: theories can be theoretically improved by reformulation. In fact, many different, in modern parlance even “incommensurable”, theories can in this view all describe the same amount of data with the same accuracy. Choosing between such theories was not perceived as being meaningless, but to a certain extent depended on taste, a matter of scientific convention.

The “appropriateness” of a theory, however, has a limited claim to reality. Thus the end-of-the-century theorising on scientific theories was, to a very large extent, based on an instrumental conception of theories with respect to observation. The American scheme was very similar to this. In a symposium in 1937, E.U. Condon made remarks almost identical to the opening sentence of Hertz’s book:

I take it to be the object of physics so to organize past experience and so to direct the acquisition of new experience that ultimately it will be possible to predict the outcome of any proposed experiment which is capable of being carried out — and to make the prediction in less time than it would take actually to carry out the proposed experiment.⁴

The crucial difference between the American and the Continental concept of a scientific theory lay in the relative evaluation of all the components of the picture. From the neo-Kantian vantage point, the “empiricism” and “pragmatism” which dominated the Anglo-Saxon environment tended to focus too much on the first two aspects of a scientific picture, while not giving proper weight to the latter. Although the explanation of phenomena was an important aspect of science, for the typical Weimar intellectual the distinguishing aspect of science was the access it provided to what lay behind these phenomena. The “understanding” of the phenomena rather than their explanation in terms of a numerical model was what defined science. From the German point of view, a purely instrumentalist or empiricist concept of a scientific theory was not inferior, but impoverished: empiricism lacked the theoretical outlook and the metaphysical basis which, in the German climate, made science interesting and worthwhile.

The point is that “appropriateness” or its equivalent was an important component of theorising for the German intellectual (as we will see in what follows, in some quarters it was given a decisive influence in determining what sort of science was “German” and “non-German”). For the Americans, by and large, theory was a means of interpreting experiment and its precise formulation was not the subject of intense philosophical speculation.

It is in the light of this difference that we have to judge the relative positions of the German and American quantum chemists.

⁴Cited in Schweber (1986), p. 65.

The effect of this environment on the development of science should not be underestimated. We will now proceed to discuss its influence in more detail.⁵

2.2. *Physics and chemistry in Weimar Germany*

The subject of the relative positioning of physics and chemistry in Weimar Germany is extremely complicated. On the one hand, the distinction between chemistry and physics had overtones of a deeper distinction, dominant in Weimar Germany, between “*Zivilisation*” and “*Kultur*”. On the other hand, this distinction was not the outcome of a rigorous philosophical attitude, but rather resulted from a confluence of Romantic and neo-Kantian tendencies, which interlocked with the dominant social structure of Weimar academia. We therefore start our exposition by describing the distinction between *Zivilisation* and *Kultur*, and then describe how the distinction between chemistry and physics was grafted onto this distinction.

2.2.1. *Intellectual culture*

The cultural climate of Weimar Germany is best shown by a characteristic distinction, or even an antithesis, between *Kultur* and *Zivilisation*, culture and civilisation. *Kultur* was associated with “*Bildung*”, a general education, preferably in the humanities, leading to a general moral and intellectual enlightenment. Its opposite, civilisation, only had the outward signs of culture. Ringer (1969) describes the difference between the two very clearly:

Zivilisation was identified with the “outward” signs of a limited sort of education. At first, it referred primarily to questions of social form. It suggested superficial polish; but it also implied a generally practical and worldly sort of knowledge. With time, the term civilization was quite naturally expanded to cover all the results of “outward” progress in economics, technology and social organisation, while *Kultur* always continued to stand for the “inner” condition and achievements of educated men.⁶

A common characteristic of many groups, both from the extreme right and the extreme left in the Weimar Germany of the twenties, was that their attitude to knowledge was determined entirely within the context of this distinction. The mathematical sciences were, almost without exception, being perceived as “civilised”. An openly hostile attitude to this sort of “intellectualism”, and with it mathematics and

⁵Some very good studies of science in Weimar Germany are available. I would like to mention especially Jeffrey Herf’s study “Reactionary modernism” (Herf 1984), which describes in detail the effect that these views had in the development of technology and engineering practices in Germany. Also, Paul Forman (1971) has traced the influence of these and similar ideas on the development of quantum mechanics. For the later period, there is Beyerchen’s book on science in the Third Reich (Beyerchen 1977), which includes a discussion of “Aryan physics”. A very good view of the academic climate in Weimar Germany is given by Ringer (1969).

⁶Ringer (1969), p. 90.

physics, prevailed. In popular culture, the intellectual was perceived as a “civilised” person, lacking insight into *Kultur*.

For instance, the writer Gertrud Bäumer wrote in 1919:

Two things characterise these intellectuals: first, their conviction that they are the salt of the earth, born leaders who appoint themselves as the mass movement’s interpreters and commentators; second, their timidity in the realm of ideas. Alienated from nature and removed from powerful emotions, these are shallow human beings who take their inspiration from ideals, from intellectualism as a sport or game.⁷

Even though Bäumer was a feminist on the left side of the political spectrum, in her view of intellectuals she joined the extreme conservatives, who also accused academics of lacking in *Kultur* while possessing rather too much *Zivilisation*.

Who, then, were these intellectuals? As Ringer (1969) has argued, the German academic class of the time is perhaps best characterised as a class of “mandarins”, highly educated officials, who, at the end of the nineteenth century and the beginning of the twentieth, formed a closed social group. The entry ticket to this group was education, preferably in the humanities. The “educated” person, it was supposed, would be in possession of a certain cultural soul, mindset and spirit, all embodied in the German word “*Geist*”. In this climate, the “utilitarian” natural sciences were seen with some suspicion, a typical French–British variety of reason that focused obscenely on material gain, and was merely “civilised”.

This attitude had its effects on the development of knowledge in Weimar Germany. As its result the predominant atmosphere was one of “*Lebensphilosophie*”, in which reason had the function of leading to a general moral and intellectual enlightenment, the development of the spirit.

Of the traditional academic subjects, mathematics, physics and to a certain extent engineering were part of “intellectualism” and thus shared in the general hostility. The humanities, the “*Geisteswissenschaften*”, had an easier task: since they were not so intimately connected with measurement and observation, it was easier to drive home the points about *Kultur* by attacking natural science. So, as a result, also in much of the humanities a hostile attitude towards the natural sciences prevailed. Othmar Spann, for instance, in his “*Kategorienlehre*” wrote:

The quantifying, so-called exact, investigation is on the contrary merely measurement and, since it ignores the essence of things and must decompose them into magnitudes in order to inventory them, it does not deserve the name *Wissenschaft* in the same high sense as the *Geisteswissenschaften*. The question of utility and achieved goals is one thing, the worth of genuine *Wissenschaften* concerned with totality and essence

⁷Bäumer (1919) in Kaes, Jay and Dimendberg (1994), p. 287.

is another. Such worth modern mathematical science does not possess today.⁸

This “measurement”, “quantifying” and “utility” was viewed with the utmost suspicion. German cultural and intellectual circles tended to stress the dehumanising aspects and cynicism of rationality and contrast it strongly with the “cultured” or “educated” point of view.

The *Lebensphilosophen* adhered to views of the existentialist and phenomenological kind. In the debate between “*erklären*” (explain) and “*verstehen*” (understand) the common wisdom was that the latter was to be far preferred to the former. “Creative” science, it was stated, should be aimed at understanding, rather than explanation. In this atmosphere, self-proclaimed intellectuals who revelled in crisis, decadence and decay and in general had an antirationalist attitude were perceived as the intellectual leaders of the day.

As a result, the natural sciences in Germany had a somewhat strained relation to the tendencies and rhetoric prevailing in German culture, to the rest of academia, especially the humanities, and even to technology. We have now illustrated the first two points. The last one, the strained relation to technology, requires further discussion.

2.2.2. *Technology*

Technology, as opposed to science, in this climate had a position entirely its own (Herf 1984). On the one hand, in this climate it was commonplace to stress the dehumanising aspects of technology. Movies such as Fritz Lang’s *Metropolis* (1927) focus extensively on the mind-numbing aspects of “rationalisation” such as practised in contemporary manufacturing methods (commonly called Americanism or “Fordism”). The destruction of human life, as effected by a hyperbola of modern society, is put in stark contrast to more “natural” values, which in this society only the rich can afford.

But it would be a mistake to think that the German intellectual climate of the day therefore had a problem with technology as such. The main problem it perceived with technology was technology’s susceptibility to the corrupting effects of money. Lang’s movie ends with a converted capitalist and the destruction of the underground factories he has constructed in his greed.

This aversion of utilitarianism found its counterpart in the relative evaluation of science and technology, for instance in the work of Spengler. Compare the following two sections from Spengler’s best-seller “*Untergang des Abendlandes*” (“Decline of the West”), the first on the relation between money and (mathematical) science:

With this goods become wares, exchange turnover, *and in place of thinking in goods we have thinking in money.*

⁸Given in Forman (1971).

With this a purely extensional something, a form-of-limit defining, is abstracted from the visible objects of economics just as mathematical thought abstracts something from the mechanistically conceived environment. Abstract money corresponds exactly to abstract number. Both are entirely inorganic.⁹

Now, for comparison, look at the following quote describing technology:

The Faustian inventor and discoverer is a unique type. The primitive force of his will, the steely energy of his practical ponderings must appear queer and incomprehensible to anyone at the standpoint of another culture, but for us they are in the blood.¹⁰

These two passages show an interesting discontinuity between science on the one hand and technology on the other.¹¹ Scientific measurement is not creative, comparable to “money thinking” and scientific reasoning is lacking in *Kultur*. It is too “intellectual”. Its opposite is technology, which is creative, unique, and incomprehensible to someone from another culture.

A similar division also appeared on the left, albeit with a different interpretation. Bertolt Brecht’s “*Das Leben Galilei*” (1938/39), strictly speaking, was written outside the Weimar period outside Germany, but it still gives us much of the typical Weimar picture of capital and physical science.¹² On the one hand, it portrays Galileo as a reckless opportunist who earns a lot of money from a telescope the design of which was obtained from a scientifically illiterate traveller to Amsterdam. The subsequent use of the telescope is both for astronomy and for trade. On the other hand, the Registrar of the university puts unrelenting pressure on Galileo to come up with something useful, thus prompting the mercantile use of the telescope. Pure science, it is asserted, does not earn money and does not win a war. Technological advance does. The picture which thus emerges is that scientific advance can take place in the midst of political and economic pressure, but is at the same time detached from this pressure. Similarly, scientific advance is to a large extent detached from technological advance, but perhaps parasitic on it.

As a result of this mindset, there appeared a very deep intellectual cleft between science and technology, with physical and mathematical science, roughly, being

⁹(Spengler 1932), p. 404.

¹⁰(Spengler 1932), p. 410.

¹¹The placement of Spengler’s ideas on science, especially his philosophy of science in the Weimar intellectual milieu, should merit an independent study. In short, Spengler’s view of science is that science has become “civilised”, has become removed from its origin and is in a state of severe intellectual crisis and decay. On the emergence of the atomic theories of Bohr and Rutherford, Spengler remarks: “If we observe how rapidly card-houses of hypothesis are run up nowadays, every contradiction being immediately covered up by a new hurried hypothesis; if we reflect on how little heed is paid to the fact that these images contradict one another [...], we cannot but realize that the *great style of ideation is at an end* and that [...] a sort of craft-art of hypothesis building has taken its place” [(Spengler 1932), pp. 215–216].

¹²The play can also be said to be a reflection on science in the Third Reich. However, science policy in the Third Reich was to a large extent a continuation of typical Weimar ideas on knowledge.

depicted as a non-creative “civilised” endeavour somewhat similar to corrupted financial speculation. Technology becomes a destructive force only when subjected to the speculative perversions of the financial markets, to “utilitarianism”. Without these, it is an expression of the “primitive force of will”, possessing “steely energy”.

Thus the dividing line seems to be located in the *numerical* aspect of inquiry—the locus of the distinction being the perception that “creative” science is not numerical science, whereas science working with mathematical formulae and numbers is not geared towards “totality and essence” but aims for an impoverished sort of “explanation”.¹³ High *Kultur* prestige thus came with science aimed at “understanding” phenomena in a humanitarian tradition, as opposed to “explanation” in terms of a mathematical model.

The interesting outcome of all this, in the end, was that it gave rise to the view that technology could do without science, that it had a dynamic of its own. This “reactionary modernism” was to become more and more important as time in the Weimar republic went by.

2.2.3. The “academic proletariat”

A few unattractive social changes tended to reinforce this negative cultural attitude towards science.¹⁴ With the country still in a state of economic and cultural shock, students tended to study the subjects that would improve future job opportunities. In the years between 1913 and 1924, mathematics and natural science lost a significant proportion of their students, while for the “technological” subjects, such as economics, chemistry and engineering, student numbers all increased.

Table 2 of Beatus (1975) shows the enrolment numbers in German universities.¹⁵ The following trends stand out. The number of chemistry students in the decade 1913–1924 quadrupled. In all, mathematics and physics lost 23% of their student

¹³It is interesting to note that in this respect, judging by the outward appearance of a discipline, reactionary modernism inverted the utilitarian–non-utilitarian distinction we currently use. “Utilitarian” (geared towards “explanation”) in this view was very close to “mathematical”, “non-utilitarian” (geared towards understanding) to “non-mathematical”. Currently, we tend to see the mathematical and theoretical sciences as “basic”, i.e. relatively far removed from practical applications.

¹⁴The following section relies to a large extent on the information collected in Beatus (1975).

¹⁵The table is given on p. 50 in the thesis of Beatus. Specifically, for the numbers interesting us here, the data are:

Major Field	1913/14	1919/20	1923/24	% increase or decrease
Law	9373	17024	22232	+137
Economics	2316	8291	12167	+448
Math and Natural Science	6502	7905	4984	–23
Chemistry	889	2936	3671	+306
Total	57171	87007	76859	+34

The relative importance of Mathematics and Natural Science thus went from more than 11% of the total university enrolment in 1913/14 to 6.5% in 1923/24.

body in this decade, while in the same period the number of law students nearly tripled, the number of economics students grew by a factor of 5 and the total population of the universities went up by 34%.

The explanation for the burgeoning numbers of Economics, Engineering and Chemistry students is that these were marketable professions in an increasingly uncertain world. It is therefore striking that Mathematics and Natural Science, which were, in a way, equally marketable, did not follow the general trend. So, in effect, the relative academic importance of Mathematics and Natural Science, measured as a percentage of enrolled student numbers, was almost halved. Although these data are not conclusive evidence for an intellectual crisis, they show that the decline of enrolment in Mathematics and Natural Science was against the general trend.

Under these circumstances the hopes of an expansion of German natural science quickly vanished. Economic problems only aggravated the situation. The inflation-corrected salaries paid out to engineers and scientists dropped rapidly by about two thirds during the inflationary crisis of 1922/23, and in fact dropped in a larger proportion than the salaries of lower-educated workers, who lost about half during the same period. On top of this, most educated circles lost all their accumulated property in the same period. Money deposited in banks, shares or trusts was virtually worthless in the course of a year, overseas travel impossible and books almost impossible to get.

Nevertheless, it is not the case that an actual “academic proletariat” existed before roughly 1928. Even after the inflation crisis, most academics would still earn about twice as much as a lower-educated worker, professors teaching the desirable subjects could still get relatively wealthy from student fees, and were mostly living above the subsistence minimum.

But it is certainly the case that academics in Weimar Germany were operating under the condition of a diminished horizon of expectations. Though the situation as such was perhaps not bad, it had gotten worse very fast. Economists and engineers were by no means exempt from diminished expectations. The low status of engineers and economists is obvious from the following exhortation to company management:

In the majority of cases we are dealing with the far too many academics (economists and engineers) who must be happy to have found any living at all. One of the most important tasks of management should be to check the unwarranted expectations of this type of employee. For example, salaries should be determined exclusively by the service which can be rendered. Addressing academics curtly and handling these mass-produced products unceremoniously can only be in the best interest of the business.¹⁶

¹⁶F. Giese: *Menschenbehandlung beim büropersonal* (“The treatment of office personnel”), *Der Werkleiter* (“The Manager”) 2, 147 (1 March 1928); quoted from Beatus (1975), p. 190.

2.2.4. *Physics and (quantum) chemistry*

What does the above material contribute to a discussion of the relative role of physics and chemistry? In my view, the existing situation, outlined above, gave rise to difficulties in the integration of the emerging quantum chemistry in the wider scientific environment of Weimar Germany.

This problematic situation came about as the result of three different trends: the placement of quantum chemistry in physics, the different perception of chemistry and physics, together with the institutionalisation of German science, and the continuous threat of an “academic proletariat”.

In the first place, as both the circumstantial and the actual evidence suggest, physics in Weimar Germany found itself in a rather dramatic situation. Paul Forman (1971), largely drawing on evidence similar to that given above, concluded that the physics community, instead of retreating into the high details of their science and entrenching themselves in their technological communities, addressed the hostility question head-on. Physicists largely copied the popular language of “culture”, “civilisation” and “*Geist*”. They even made concessions to the popular point of view, in presenting the quantum concepts of “causality” and “uncertainty” largely in line with a prevailing cultural mood of crisis, collapse and decay.¹⁷ Forman’s suggestion is not so much that the Weimar culture influenced the very content of the physics developed in it, but that it did influence the language in which this content was presented, especially in popular lectures.

My suggestion, in opposition to Forman, would be that the behaviour of the physics community was largely one of entrenchment, but it was entrenchment in the existing vistas of German academia, reactionary modernism and conservatism. By citing Goethe and Schiller in their popular lectures, the German physicists made (or tried to make) it clear that they were educated too, that they were concerned with real “*Wissenschaft*”, not — heaven forbid — with “utilitarianism” or “empiricism”.

This provides a sociological clue to the embedding problems of quantum chemistry. The placement of the emerging discipline of quantum chemistry in the context of a discipline deeply in crisis mood was merely the start of the problem. The way out of this crisis mood (into the existing vistas of academia), followed by the quantum physicists, by and large did not exist for the physicists constituting the emerging quantum chemistry community.

The lesser reason for this is demographic: by and large, the founders of quantum chemistry were members of a somewhat younger generation than the founders of quantum mechanics. As a result, they tended to have a lower academic status and the likelihood of being invited for a popular lecture was smaller for quantum chemists than for quantum physicists. London, Heitler, and many more of the men whose papers have been collected here were, at the time of their writing, “*Privatdozent*”. This was a not very enviable position at the bottom of the German

¹⁷On the other hand, one sometimes wonders if the ploy really worked. We bring to mind Spengler’s remarks on “card-houses of hurried hypotheses” covering up inconsistencies.

academic ladder. Pay depended immediately on the number of lectures one gave and on the number of fee-paying students visiting these lectures. The most popular (or compulsory) courses would almost invariably be taught by the higher-ranking full professors, and *Privatdozente* often got stuck with the electives. Thus, for someone in this position, pay was neither very good nor very regular.

More important was the different perception of chemistry and physics existing in Weimar Germany. To my knowledge, there are no studies on the role of Weimar Republic chemistry in reactionary modernism. But my suggestion would be: following on from the different perceptions on “understanding” and “explanation” the engineering and chemistry professions had a higher *Kultur* prestige than Mathematics and Natural Science.

Quantum chemistry as it emerged in the physics community thus found itself in the wrong place at the wrong time. The enrolment numbers suggest a context wherein the popularity of chemistry on the one hand and mathematics and physics on the other had very different trends. Chemistry, in this respect, followed the trend of economics and engineering. As we have argued above, technology more easily aligned itself with the paradigms of *Kultur*, leading to a rather large intellectual barrier between mathematical science on the one hand and technology on the other. Stated bluntly, the technological programme of reactionary modernist right wing Germany was one that supposed it could do without science; it supposed that technology had a dynamic of its own. It still remains to be seen how far the German chemists supposed they could do without the information of quantum physics.

Possibly as a result of this problematic relation with “technology”, physicists’ contacts with chemists in Germany were largely coincidental and no long term research programmes on a sustained common basis took place.¹⁸ It was probably easier to bridge the gap between chemistry and physics by welcoming chemists from the USA (where these differences were not so sharply defined) than by addressing the German chemists immediately. From the chemists’ perspective, an alignment with quantum chemistry would mean that the long-cultivated distrust of “utilitarian” disciplines had to be overcome. It would also make an undesirable alignment with “quantitative science” more clear.

On top of this, German science was organised in a heavily institutionalised form, with the barriers between institutions almost impossible to overcome. Already this circumstance made the development of quantum chemistry almost impossible in the German context, notwithstanding the fact that the institutional barrier was strengthened by a cultural barrier as well.

As a result, from its inception, in Weimar Germany quantum chemistry had a problematic position. Such conditions as described above were far from optimal

¹⁸It is for instance interesting to note that almost all papers collected in this volume were published in the *Zeitschrift für Physik*. The *Zeitschrift für Physikalische Chemie*, even the section dealing with atomic theory and spectroscopy, carries almost no articles by quantum chemists in the period covered here. Herzberg, in so far as he can be called a quantum chemist, is one of the few exceptions.

when it came to starting a new research programme, especially one that, for its survival, depended heavily on overcoming institutional barriers. In my opinion, this situation does explain such facts as that Heitler and London never really followed up on their paper on the hydrogen bond, explaining other chemical bonds as well. It also explains much of the background of the sometimes existing tension between the German physicists and the American post-doctoral fellows who came to study quantum chemistry in Germany.

Much later, Fritz London would comment on the differences between the chemical and the physical approach to quantum chemistry, in a way which was perhaps not very complimentary to the chemists, but which shows some of the old antagonisms long cultivated in Germany.

The word “valence” means for the chemist something more than simply forces of molecular formation. For him it means a substitute for these forces whose aim is to free him from the necessity to proceed, in complicated cases, by calculations deep into the model. It is clear that this remains wishful thinking. Also the fact that it has certain heuristic successes. We can, also, show the quantum-mechanical framework of this success. . . the chemist is made out of hard wood and he needs to have rules even if they are incomprehensible.¹⁹

The Weimar republic ended with Hitler’s rise to absolute power in 1933. The Jewish intelligentsia quickly lost their academic posts, and as a result, many of the original physicists who made up the German quantum physics and chemistry community had to seek refuge abroad.

With Hitler’s ascent to power, the “reactionary modernist’s” concept of technology gained the upper hand. It was characteristic of this era that the Nazis strived to construct an “irrational technology”, to combine “culture” and “technology” into what Goebbels would call “*stählernde Romantik*”, a romanticism of steel.²⁰ For the Nazis, the quantum chemistry community, even if many of its best members had not been Jews, was undoubtedly too “civilised”, too “scientific”, to be palatable. Much of this was to the detriment of German science, as is for instance argued by Goudsmit in his later study of the German failure to create the atomic bomb (Goudsmit 1947). Goudsmit identifies three main reasons for the German failure, which are all related to the mindset discussed above: (1) complacency, the inherent belief that German science was superior; (2) lack of interest in “long-haired” (basic) science; and (3) the intrusion of (Nazi) dogma and bad administration. With the exception of the last point, these are inherent components of reactionary modernism: German superiority, fuelled by the superiority of the German *Kultur*, would make a genuine interest in science unnecessary.

¹⁹Cited in Gavroglu (1995), p. 85.

²⁰This term is sometimes also translated as “steely romanticism”. In my view, the context of the remark makes the translation “romanticism of steel” more appropriate: Goebbels hints at the new form of romanticism that results from the modern factory or the machine of war. The remark is typical for a reactionary modernist view on technology.

The evidence suggests that quantum chemistry had failed to make a lasting impression on the German chemistry community. As a result, quantum chemistry (and quantum mechanics) all but vanished in Germany during the Third Reich. Quantum chemistry had to find a new home. This new home would be the United States.

2.3. *The atmosphere in the USA*

After this somewhat elaborate sketch of the atmosphere in Weimar Germany, we can be quite brief on the situation in the USA. The emergence of quantum chemistry in the USA falls outside the scope of the present set of translations and is also already documented very well by Nye (1993) and Gavroglu and Simoes (1994). The most comprehensive discussion of the American context of science is given by Schweber (Schweber 1986).

In almost all aspects of importance to the further development of quantum chemistry, the atmosphere in the USA was opposite to that prevalent in Germany. Technology and science were much more closely linked, there was no rampage of top-heavy metaphysical ideas on *Kultur*, and perhaps most important, there were no strong institutional barriers.

The USA was a country perhaps best characterised by its pragmatism, dominated by an “empiricist temper regnant” (Schweber 1986). Several studies have stressed the pragmatic attitude of nineteenth century America, and the concurrent pragmatic attitude towards “theory”. Many theorists, such as Mulliken and Slater, did an experimental PhD and only then, during their stays in Germany as post-doctoral researchers, did they familiarise themselves with quantum theory. In this atmosphere, theory and experiment were therefore closely related, with a specific task designed for the theorist: theories should be used to calculate the outcome of experiments, rather than lead to “quibbles about words”.

Another factor increasing the acceptance of quantum chemistry in the USA was the institutional context. There were few, if any, special theoretical departments before 1900; after that, the number of theoretical departments multiplied. The theoretical aspects of many experiments were too much to handle for many experimentalists, so the need to bring in specialised theorists to support the interpretation of the experiments was recognised and acted upon.

This origin served very well to inhibit the development of institutional barriers which might otherwise have arisen. Whereas on the Continent, theorists and experimentalists were part of different groups, in the United States theoretical science developed in close collaboration with experiment, and theorists were often part of, or working in very close collaboration with, experimental groups. This must have led to a considerable number of informal communication channels, which helped to align quantum chemistry quickly with its subject matter.

Furthermore, many of the visiting scientists who learned quantum mechanics in Weimar Germany on post-doctoral appointments, had originally trained in

chemistry. As a result, quantum chemistry could become a true part of chemistry and physics, something which was almost impossible in Germany.

The American quantum chemistry community developed very quickly. As Dresden (1992) pointed out, this could be due to the fact that many of the founders of American quantum chemistry had a very similar development, leading from “an early exposure to preliminary quantum theory via a substantial apprenticeship in formal quantum mechanics to a notable success in atomic and molecular structure” (page 28). This common path of development helped enormously to create a well-trained, coherent quantum chemistry community in the USA.

2.4. The embedding of quantum chemistry

We will now draw some tentative conclusions on the social embedding of quantum chemistry in Germany and the USA, focusing on the aspects of genealogy, physical homeland, external recognition and shared values.

As we have seen, in Weimar Germany quantum chemists were predominantly physicists; in contrast, in the USA, they tended to be chemists. So, in the genealogy aspect, quantum chemistry originated as a branch of physics rather than chemistry, and was taken into the chemical environment (not without some problems!) by the American scholars who visited Germany in the twenties.

As a result, core literature and practices initially were taken from physics rather than chemistry. In some instances, this led to attempts to construct an overarching theory, embracing all chemistry. Especially, Heitler got in trouble more than once. Remarks such as “We can, then, eat chemistry with a spoon”²¹ did not go down very well, not even with colleagues:

Wigner used to tease him, since he was sceptical that the whole of chemistry could be derived in such a way. Wigner would ask Heitler to tell him what chemical compound between nitrogen and hydrogen his theory could predict, and “since he did not know any chemistry he couldn’t tell me”.²²

So, as a result, quantum chemistry became a discipline of “applied quantum physics”, a field in which accurate applications were muddy and required quite a bit of compromise.

It is telling to a large extent that some of the more prominent, but not all, of the physicists who founded quantum chemistry²³ later in life went on to other subjects, leaving quantum chemistry to the chemists.

Due to the cultural differences existing between physics and chemistry the physical “homeland” of quantum chemistry in the Weimar Germany context amounted

²¹Letter from Heitler to London, cited in Gavroglu (1995), p. 54.

²²Both these remarks are given by Gavroglu (1995), p. 54.

²³Notably London, Heitler, Wigner and Oppenheimer. Many of those who stayed in quantum chemistry belonged to the group of American post-docs who had visited Germany in the twenties. To this group belong Pauling, Mulliken and to some extent Slater.

to little more than a variety of “applied quantum physics”. With the lack of a distinct homeland came the lack of external recognition. So, on this set of criteria, we suggest that quantum chemistry as a separate discipline was never very well embedded in the Weimar academic milieu. From the viewpoint of the physics community, it was seen as a branch of “applied physics”; from the chemists’ point of view, merely as a branch of physics.

In contrast, in the USA institutional barriers were not so strong. As a result, a fruitful cooperation between chemists and physicists was possible from the start, and even though a “homeland” was initially lacking, there was a distinct possibility of creating it. Dresden’s remark on the common “school” of the early quantum chemists comes to mind: the genealogy of quantum chemistry, in so far as it was not already present, was in the making here.

3. The intellectual core of quantum chemistry

We have, up to now, argued that the social and intellectual circumstances in Weimar Germany were, relative to the USA, not conducive to a fruitful development of the new discipline of quantum chemistry. We will now discuss some of the scientific and methodological problems that were discussed in chemistry and the way in which the emergence of quantum chemistry addressed these problems.

3.1. *Realism: the mechanical dream*

Much of the continental philosophy of chemistry and physics was a variety of the sort of conventionalism which we discussed above. We have pointed out already that physics and the philosophy of physics were, on the continent, much more continuous disciplines than they are in academia today.

Therefore one of the first issues in the intellectual core of quantum chemistry is realism. Perhaps a little surprisingly, realism did not lead to spirited debates among quantum chemists.

The *philosophy* of continental nineteenth century chemistry was, like nineteenth century physics, dominated by discussions on the “reality” of scientific entities. In the case of chemistry these were notably atoms; in the case of physics, the discussion focused on the “reality” of the terms appearing in the physical laws. One of the physicists of the older generation, Ernst Mach, entered a fierce debate with Planck on the issue of realism. According to Mach, “atoms” were mere instruments in scientific theorising, and it was as useless as it was senseless to describe them as “real”. Physics had become a religion, complained Mach, drawing conclusions far beyond what is warranted by observation and sensible theorising:

One sees that physicists are already on the best way to becoming a church and have already grasped the readiest means at hand. Let me answer plain and simple: If belief in the reality of atoms is so essential to you, then I will have nothing to do with physical ways of thinking;

I will no longer be a genuine physicist; I will give back my scientific reputation. In short, thank you so much for the community of believers, but for me freedom of thought is more precious.²⁴

The conventional idea, taken over from the neo-Kantians, was that we cannot say with certainty what goes on beyond the phenomena, even though we conceive mechanisms that allow us to connect these phenomena. This is very similar to, for instance, the Hertzian view of science discussed above in which, in the end, the appropriateness of a theory has only a very limited claim to reality. The purpose served by theorising was the connection of events and observations.

The chemists fully adhered to this view of theory or “pencil and paper chemistry”.²⁵ The explanations in terms of atomic theory were successful, popular, and “disbelieved in realist terms”.²⁶

At the turn of the century, the question of the “reality” of atoms was not solved, but most chemists were going along with the idea that atoms were a useful concept in chemistry. As a result, some chemists started working on theories of chemical valency, attempting to explain valency as a property of the inner structure of the atom.

In a certain sense, the question of the reality of atoms was therefore displaced by the question of what constituted a valid chemical explanation in terms of atoms. In the nineteenth century, atomic theory had the shortcoming that it was not furnished with a suitable mechanics, a theory of what went on inside the atom.²⁷ As Nye (1993) has stated, a mechanical explanation of the behaviour of atoms was the “elusive dream” of chemistry. Before quantum chemistry, and to a large extent even after its rise, this dream was not “relinquished; rather, it was repressed” (page 71).

3.2. *The intruder: spectroscopy*

Bohr’s early quantum theory posed some new problems in the mechanical explanation of chemistry. In Bohr’s theory, the electrons move in circular or elliptic orbits around the nucleus, and thus are in a dynamic equilibrium. The fact that most molecules have fixed structures led chemists to believe that a dynamic equilibrium in atoms could not in reality exist. In many of the chemical models, the electric charges had fixed positions in space.

Bohr early on tried to solve chemical problems with his model, but the chemical explanations Bohr was able to offer (notably a model for the chemical bond and a relation between the placement of elements in the periodic table and their electronic

²⁴Blackmore (1992), pp. 138–139.

²⁵Nye (1993), p. 69.

²⁶Nye (1993), p. 70.

²⁷Casimir (1983) has summarised the situation poignantly by stating that at the end of the nineteenth century, the situation was that the existence of the atom was under debate, but (if the atom existed) its mechanical theory was supposed to be known (namely classical mechanics); instead, at the beginning of the twentieth, the reality of atoms was a fact, but the mechanics of the atom was unknown.

configurations) were not as successful as Bohr's achievement in spectroscopy: the explanation of Balmer's law. As a result, spectroscopy became an important field guiding the development of early quantum mechanics.

This prominence of spectroscopy, which originated in the "old quantum theory", would also cause a sometimes fierce debate between the two rival ways of explaining the structure of the chemical bond.

Especially for Hund and Mulliken, molecular spectroscopy would become an important guiding principle in the development of theories of the chemical bond. Mulliken's "pragmatic" approach calculates the energies of the hydrogen molecule through addition of an electron to the hydrogen molecule ion. (Also Hylleraas follows this procedure in his paper on H_2 translated in this volume, although his description of H_2^+ is based on an elliptical coordinate system.) There can be little doubt that Mulliken's aim was the development of a molecular spectroscopy, not the development of a theory of the chemical bond. From this perspective, the natural choice, as indeed Hund and Mulliken made it, is to see the molecule as a collection of nuclei fixed in certain spatial positions with an additional electron cloud surrounding these nuclei. So the method they devised is applicable to the chemical bond. It pictures the electrons as each occupying a "molecular orbital" which in extent stretches over the whole of the molecule. In this way, the chemical bond results as the effect of the atoms losing their identity to a large extent, since they start, in a certain way, to "share" electrons.

3.3. *The dream revisited: valency*

In opposition to what would later become the "molecular orbital" theory, the paper by Heitler and London started from the concept of chemical valency, and was an attempt to explain the chemical bond by using properties of the atoms individually. The paper describes the interaction between two individual hydrogen atoms and the chemical bond appears as the result of a quantum-mechanical "resonance". Heitler and London's paper is generally seen as the first paper giving a quantum-mechanical description of the chemical bond and the behaviour of the noble gases. It describes these effects as a pure quantum-mechanical phenomenon. But what was still lacking in this picture was the explanation of "directed valencies". This addition would only be made by Slater and Pauling. The Heitler–London method was difficult to apply to more complicated molecules, because it started from the assumption that the individual atoms would retain their properties in the molecule to a large extent.

The Mulliken–Hund approach would, when quantum chemistry (so to speak) "emigrated" from Europe to the USA, gain the upper hand. The fact that Hund and Mulliken were coming to the fore as the first to describe the chemical bond drew quite a lot of criticism from London in 1935, when he started a renewed interaction with Heitler. This episode is described in a lively manner in Gavroglu (1995). A problem is that Heitler and London never followed up their paper by presenting

a wider application to chemistry, but only treated H_2 and the interaction of He atoms. In this later stage, they did consider, perhaps not for very long, treating other cases. But by then it was too late for London and Heitler to get back into quantum chemistry.

3.4. Applications

In Germany in the twenties and early thirties, quantum chemistry was closer to applied quantum mechanics (physics) than to theoretical chemistry. It was by and large the Americans, Slater and especially Pauling, who stressed the chemical applications of quantum theory and were prepared to sacrifice some degree of exactness for applicability. Chemistry could only be fitted in a quantum-theoretical scheme by making (sometimes rather large) simplifications. This often led to harsh criticism, of the sort for instance expressed in the private communications between Heitler and London.

What we have pointed out so far is that the Americans and the Germans in the quantum chemistry community in the twenties and early thirties of this century differed not only strongly in cultural background, but also in conceptual outlook. The Germans, by and large, originated from an environment in which a mechanical theory of the chemical bond, which is what the emerging quantum chemistry had to offer, had long been an elusive dream. The emerging quantum chemistry in Germany is therefore perhaps best characterised as “applied quantum mechanics” rather than as “the theory of the chemical bond”.

On their side, many Americans were not very interested in a “theory” of the chemical bond as such, but rather in its explanatory power. For most of the Americans, theory was a means of adding an interpretation to experimental data, or, as Slater was to put it later:

A theoretical physicist in these days asks just one thing of his theories: if he uses them to calculate the outcome of an experiment, the theoretical prediction must agree, within limits, with the results of the experiment. He does not ordinarily argue about philosophical implications of his theory.²⁸

From the continental point of view, such a method seemed far from ideal. Gavroglu (1995) quotes Hund as saying: “Mulliken’s paper is rather American, e.g. he proceeds by groping in an uncertain manner, where one can decide theoretically the cases for which a particular claim is valid” (page 89). In his autobiography, Mulliken sums it up when he describes the reason for visiting Germany in 1927:

I had no special program in mind, but planned to talk with spectroscopists and theorists about the problems of molecular structure and

²⁸J.C. Slater, “The electrodynamics of ponderable bodies”, cited in Schweber (1990), p. 391.

spectra, especially with Hund, and perhaps to do some writing. Probably I ought to have devoted more attention to an intensive study of quantum mechanics, but I was satisfied with a general knowledge of its methods and principles sufficient to help me understand particular molecules or types of molecules and their properties; especially their spectra. In short, I was more interested in getting acquainted with molecules than with abstract theory about them.²⁹

With this in mind, it is little surprise that the American quantum chemists were sometimes willing to engage in simplifications of the “applied quantum physics” theories that their continental colleagues abhorred. On top of this, in the success that followed Pauling’s papers on the chemical bond, the work of Heitler and London was becoming the less favored approach to the description of the molecular bond. In 1935, this gave rise to a situation in which Heitler and London, now both relatively isolated in Great Britain while the scene of the action had moved to the USA, “tried to save what could not be saved” [Gavroglu (1995), page 82]. Some of the old antagonisms to chemistry were revived (see the quotation before) but, all in all, Heitler and London found themselves in a hopeless situation as far as quantum chemistry was concerned.

4. Conclusion

Most of the papers collected in this volume were written before quantum chemistry existed as a branch of *chemistry*. Quantum chemistry as a “theory of the chemical bond” was in Germany perceived mainly as “applied quantum mechanics”. As such, it was a section of the physics departments, its practitioners were mainly physicists, they published mainly in physics journals, and in many cases in later life went on to do physics. The papers were written under a cloud of not very enviable material, social, cultural and even intellectual circumstances. Nevertheless, all papers stand out for attention to experimental detail and clarity of style.

Though the arguments presented in this essay are not conclusive, I hope to have made it plausible that the smooth transition of quantum chemistry to the USA, as it took place in the 1930s, had to do with the embedding of the quantum chemistry community in the wider environment in Weimar Germany, and the manner in which the application of quantum mechanics was ill-suited to the Weimar intellectual environment.

The papers presented in this book form a significant portion of the German origin of quantum chemistry. Now that we have outlined the background from which they were written, we hope to have added to the reader’s understanding of some of the finer points and to help the reader understand the particular style of the argument.

²⁹Mulliken (1968), p. 59.

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