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Quantum mechanical atom models, legitimate explanations and mechanisms

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Abstract
The periodic table is one of the best-known systems of classification in science. Because of the information it contains, it raises explanation-seeking questions. Quantum mechanical models of the behaviour of electrons (which describe an electron configuration for each kind of atom) may be seen as providing explanations in response to these questions. In this paper we first address the question 'Do quantum mechanical models of atoms provide legitimate explanations?' Because our answer is positive, our next question is 'Are the explanations provided by quantum mechanical models of atoms mechanistic explanations?'. This question is motivated by the fact that in many scientific disciplines, mechanistic explanations are abundant. Because our answer to the second question is negative, our last question is 'What kind of explanation do quantum mechanical models of atom provide?' By addressing these questions, we shed light on the nature of an important type of chemical explanation.

Keywords Mechanistic explanation · Periodic table regularities · Physical dependency · Structural explanation · Unification

Introduction

The periodic table is one of the best-known systems of classification in science. In 1869 the Russian chemist Dimitri Mendeleev stated in a presentation to the Russian Chemical Society that there is a relation between the chemical properties and the atomic weights of the elements. If the chemical elements are ordered according to the atomic weight the chemical properties of elements appear to reoccur after certain definite intervals: the properties exhibit periodicity. Since 1869, over 700 different versions of the periodic table were published (Scerri 2007, p. 20). Contemporary versions of the periodic table differ in important respects from those in the nineteenth century. However, they share an important property: they encode information about which elements display similar chemical behaviour.

Because periodic tables encode information about similar behaviour, they raise explanation-seeking questions. Quantum mechanical models of the behaviour of electrons (which

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describe an electron configuration for each kind of atom) may be seen as providing explanations in response to these questions. In this paper we first address the following philosophical question:

> Do quantum mechanical models of atoms provide legitimate explanations?

Because our answer is positive, we address a further question:

> Are the explanations provided by quantum mechanical models of atoms mechanistic explanations?

This question is motivated by the fact that in many scientific disciplines, explanations of regularities are mechanistic.

Because our answer to the second question is negative, we address a final question:

> What kind of explanation do quantum mechanical models of atoms provide?

By addressing these questions, we shed light on the nature of an important type of chemical explanation. In a recent paper on explanation and the periodic table, Lauren Ross writes:

> In modern chemistry, scientists frequently appeal to atomic structure in explaining the chemical and physical properties of the elements and their periodic character. (2021, p. 84)

She supports this claim by quoting several chemistry textbooks (2021, pp. 88–89). In this paper we scrutinize this explanatory practice in chemistry by means of our three philosophical questions.

Our paper starts with two sections that set the stage. In the "The periodic table and the explanation-seeking questions it raises" section we discuss the periodic table and the explanation-seeking questions it raises. In the "Potential explanations for chemical regularities: quantum mechanical atom models" section we present the potential explanations: the quantum mechanical models of the structure of atoms. In that section we provisionally call these models 'accounts', because at that stage in the paper we want to stay neutral as to their explanatory value. In "Mechanisms and mechanistic explanation" and "Physical dependency and why it matters for explanation" we present the main philosophical tools that we need to answer the three philosophical questions: the essentials of the mechanistic view on scientific explanation, and the idea of physical dependency as a requirement for explanations. In the "Do quantum mechanical atom models (electronic configurations) provide legitimate explanations?" section we address the first question above. The two others are addressed in "Quantum mechanical models do not provide mechanistic explanations" and "Structural explanations and structural unification" respectively. In "Some comparisons" we compare our results with the views defended by Lauren Ross in the paper mentioned above, and with other relevant contributions (Woody 2014, Scerri 2020).

The periodic table and the explanation-seeking questions it raises

We first give relevant information about the (history of) the periodic table ("The periodic table in the nineteenth century" and "The periodic table in the twentieth century" sections) and then clarify the explanation-seeking questions that emerge ("Explanation-seeking questions" section).

The periodic table in the nineteenth century

In his 2007 book *The Periodic Table: its Story and its Significance* Eric Scerri discusses the six discoverers of periodicity. The leading discoverer is Dimitri Mendeleev (1869). His version of the periodic system had by far the greatest influence on chemistry at his time and still today. The main organizational principle of his periodic table was the atomic weight of elements. Stephen Brush formulates the core idea as follows:

> The periodic law (as formulated in the nineteenth century) states that when the elements are listed in order of atomic weight, properties such as valence will recur periodically – for example, after seven elements. (1996, p. 599)

This central organizational principle enabled Mendeleev to design a two-dimensional classification of the elements known at his time. Ordered according to atomic weight the elements Li, Be, B, C, N, O, and F were put in the first column. Since the next known element Na was chemically similar to Li, Mendeleev put Na in a new column, next to Li (the columns in Mendeleev's table are rows in contemporary tables).

At the end of the nineteenth century, the noble gas argon was discovered by Lord Rayleigh and William Ramsay. The discovery of helium, krypton and xenon followed soon thereafter. Suddenly, a whole group of elements was discovered without being predicted by the periodic table. The noble gases formed a serious threat for Mendeleev's system. At first, Mendeleev denied that argon and helium were new elements, as he would not accept elements to be completely inert. In 1900 Ramsay suggested to Mendeleev that argon and the other noble gases should be added as a new group. This led to the version of the periodic table that is familiar to many people: the one with eight groups. (Scerri 2007, p. 156).

Mendeleev's final ideas on periodicity can be summarised as follows:

i. Ordered according to atomic weight, there is a repetition of chemical properties.
ii. There is a constant period length.
iii. Every period contains 8 elements.
iv. If there is an empty space, this predicts a yet unknown element.

Scerri compares this to a musical scale: a returning note, denoted by the same letter, sounds like the original note, but is not identical to it, being an octave higher or lower (2007, p. 18).

The periodic table in the twentieth century

Since Henry Moseley, the periodic table is no longer ordered according to atomic weight, but by atomic number. Moseley showed that certain characteristics of X-ray spectra correlated with the atomic number, but not with the atomic mass. Therefore, he proposed the atomic number as a more basal property of an element than the atomic mass (1913, 1914). In the Rutherford atomic model (developed between 1911 and 1920) an atom has a nucleus with a positive charge equal to the total number of positively charged protons in the nucleus (the neutrons in the nucleus are neutral). The atom as a whole is electrically neutral, thus the number of positively charged protons (p) is equal to the number of negatively charged electrons revolving around the nucleus (e). Thus, the atomic number $Z=p=e$. This new ordering principle solved certain problems with Mendeleev's table (e.g. the four pair reversals) and provided a more natural ordering principle.

Empirical evidence showed that the periodicity, unlike notes on a Western musical scale, is neither constant nor exact. The length of a period varies and the elements within any column of the periodic table are not exact recurrences of each other. The periodic table as it is standardized by IUPAC (the International Union of Pure and Applied Chemistry) is organized in 18 vertical groups and 7 horizontal periods. This systematization follows the ordering according to increasing atomic number.[1] The first period contains two elements, the second and third each contain eight, the fourth and fifth contain eighteen and so on. This means that Mendeleev's original ideas (ii) and (iii) are not retained: in the IUPAC table the period length is not always eight and is not constant.

Moreover, even though there is a neat ordering according to atomic number, the visual representation shows a certain discontinuity: in the first, second and third period there are no similar elements for elements in group 3 to 12. This means that the original idea (iv) is not retained either. Only Mendeleev's idea (i) remains, albeit in a more approximate nature.

Explanation-seeking questions

We can now proceed to the next step: show that there are explanation-seeking questions that can be raised.

In Mendeleev's first table, elements with similar properties were arranged in the same horizontal rows. In the IUPAC periodic table these elements are vertically ordered and are numbered from 1 through 18. Horizontally, the atomic number Z of elements increases from one period or row to the next. The arrangement of the elements is a visualization of the fact that the chemical elements exhibit a certain repetition in their properties, such as:

Elements of group 1 in solid state are good electrical conductors.
Elements of group 17 easily form compounds with elements of group 1.
Elements of group 18 do not form compounds (with the exception of certain artificially synthesized compounds).

Group 1 contains the alkali-metals, Group 17 the halogens and Group 18 the noble gases. Artificial compounds are ones that require human intervention. Until 1962, the generally accepted view was that noble gases did not form any chemical compounds at all. Hence, they were called 'inert' gases. We now know that compounds with gases of group 18 can be synthesised under specific circumstances (e.g. high pressure or low temperature). However, compounds with elements of group 18 do not occur outside of these artificial conditions.

There are many more such regularities but the three examples above suffice for this chapter. Each one leads to an explanation-seeking question:

Why are alkali-metals in solid state good electrical conductors?
Why do halogens easily form compounds with alkali-metals?
Why do noble gases only form compounds under artificial conditions?

These explanation-seeking questions are requests for explanations of regularities. We use the term 'periodic table regularities' as label for the type of explanandum involved, since the regularities use the groups of the standard IUPAC version of the period table.

[1] See www.iupac.org; the last version currently available is dated 1 December 2018.

The periodic table regularities presuppose the truth of more specific regularities, such as:

Lithium in solid state is a good electrical conductor.
Chlorine easily forms compounds with sodium.
Helium is not present in compounds formed outside of artificial conditions.

These regularities are about one type of atom, not about groups. We call them 'physico-chemical behaviour regularities' so that we can keep them apart from 'periodic table regularities'. In our discussion of the explanatory power of quantum mechanical models we will consider both levels of generality. We will use 'chemical regularities' as umbrella term that covers both types.

Potential explanations for chemical regularities: quantum mechanical atom models

We sketch the core ideas of the relevant quantum mechanical models ("Orbitals, shells, and electron configurations" section) and then indicate which regularities they may explain ("Electron configurations as explanations?" section). We also prevent some possible confusion ("An important clarification" section).

Orbitals, shells, and electron configurations

Models of atoms as we find them in quantum mechanics may account for the many chemical regularities that have been empirically discovered. A core idea of the contemporary model of atoms is that atoms consist of a dense positively charged nucleus and electrons that are clustered around this nucleus. We owe this idea to Ernest Rutherford's work in 1909–1911. Another core idea of Rutherford, viz. that the electrons revolve in orbits around the nucleus like planets around the sun, did not survive. In the quantum mechanical models, the behaviour of electrons is characterized mainly in terms of *orbitals*. Given the indeterministic nature of quantum mechanics, it is impossible to predict the exact location of an electron. However, one can determine a spatial region in which the electron is present with a certain probability (e.g. a region in which the electron is present with 0.9 probability, i.e. a region in which the electron is present 90% of the time). Such regions are called orbitals. Each electron occupies an orbital and there can be no more than two electrons in the same orbital. The two words (orbit – orbital) are very similar, but the shift indicates a radical change in how electron motion is regarded: there is no definite trajectory anymore (Scerri 2007, p. 24).

By saying that an electron occupies an orbital, we say something about where the electron is located:

– Each orbital is at an energy level, which can be determined by the principal quantum number n (the energy level associated with the most probable distance of the electron(s) in the orbital to the nucleus);

- Each orbital also has a shape determined by the angular momentum quantum number ℓ (the second quantum number);
- Each orbital also has a spatial orientation, determined by the magnetic quantum number m_ℓ (the third quantum number).
- Energy levels are denoted by natural numbers ($n = 1, 2, 3, \ldots$) while the shapes of the orbitals (determined by ℓ) are denoted as *s, p, d* and *f*.

Electron configurations as explanations?

Electron configurations can be used and have been used as starting points of accounts of the periodic table regularities mentioned in the "The periodic table and the explanation-seeking questions it raises" section. We give a brief sketch for the examples in the "Explanation-seeking questions" section:

- The elements of group 1 have an electronic configuration with a single electron in the highest energy level; the rest of the configuration is like that of the preceding noble gas. This outlying electron is relatively free to move about. This accounts for their electrical conductivity.
- The electronic configuration of elements of group 17 is such that they need only one more electron to form a closed shell. Since the acquisition of an extra electron is energetically favourable, these atoms are very reactive. They can obtain the required electron easily from elements of group 1, since these have outlying electrons.
- The elements of group 18 are atoms with a closed-shell structure: their outer shell is completely filled. As a result, these atoms are stable and have very low reactivity.

The philosophical question is: are these accounts legitimate explanations? This question is addressed in the "Do quantum mechanical atom models (electronic configurations) provide legitimate explanations?" section.

Electron configurations can also be used as starting points for more specific accounts which address a 'physico-chemical behaviour regularity':

- Lithium has an electron configuration with a single electron in the highest energy level. This outlying electron is relatively free to move about. This accounts for the electrical conductivity of lithium.
- The electronic configuration of chlorine is such that it needs only one more electron to form a closed shell. Since the acquisition of an extra electron is energetically favourable, chlorine atoms are very reactive. And they can obtain the required electron easily from sodium atoms, since these have outlying electrons.
- Helium atoms have a closed-shell structure: their outer shell is completely filled. As a result, these atoms have very low reactivity.

Again, the philosophical question is whether these accounts are legitimate explanations. This question is also addressed in the "Do quantum mechanical atom models (electronic configurations) provide legitimate explanations?" section.

An important clarification

Electron configurations obey three principles: the Aufbau principle (with the associated Madelung rule), Hund's rule, and Pauli's exclusion principle. Note that it is not the explanatory value of these principles that we are investigating here in this article. Eric Scerri argues that these principles do not explain electron configurations:

> It emerges that all three of these principles are essentially empirical, and none of them has been strictly derived from the principles of quantum mechanics. Pauli's principle, for example, takes the form of an additional postulate to the main postulates of quantum mechanics. […] So, rather than providing an explanation for electronic configurations, the three commonly used rules are really statements that summarize what is known to happen from experimental data on atomic spectra. (2007, p. 233–234)

This view is compatible with the argument we develop here, because electron configurations (as described in atom models) are part of the alleged explanans, they are not the explanandum. The question we address is not whether electron configurations can be explained by the main postulates of quantum mechanics (via the three principles). The question is: do electron configurations explain chemical regularities? And if so, are these explanations mechanistic?

Mechanisms and mechanistic explanation

Because we want to answer the question whether these explanations have a mechanistic format we provide background information on the mechanistic view on explanation. We clarify what mechanisms are ("Mechanisms" section), what mechanistic explanations of regularities are ("Mechanistic explanation" section) and give an example ("Mechanistic explanation of regularities: an example" section).

Mechanisms

We adopt the following definition of mechanisms:

> A mechanism for a phenomenon consists of entities (or parts) whose activities and interactions are organized so as to be responsible for the phenomenon. (Glennan & Illari 2018, p. 2)

Clarifying comments on this definition can be found in Chapter 2 of Glennan's *The New Mechanical Philosophy*, the book in which this definition first appeared. Mechanisms are compounds (they are composed of simpler things) and they are determinate particulars (they exist somewhere in the world).

The chapter also clarifies the key terms used in this definition. For instance, Glennan writes:

> Grammatically, entities are referred to by count nouns (or sortals). Examples of entities include proteins, organisms, congressional committees, and planets. Entities are, in a sense we will explore later in this chapter, objects—things that have reasonably stable properties and boundaries. Activities on the other hand are referred to by

> verbs. They including anything from walking to pushing to bonding (chemically or romantically) to infecting. They are a kind of process—essentially involving change through time. (2017, p. 20)

The difference between activities and interactions is clarified by Glennan as follows:

> As I understand it, the term "interaction" implies some relation between more than one entity (actors, agents, patients), while some activities can be done on their own. Daydreaming is an activity, but not an interaction, while having a conversation is an interactive activity. (2017, p. 21)

Finally, the meaning and importance of organisation is explicated as follows:

> Mechanisms behave as they do because of the organized activities and interactions of their parts. The purport of the term "organized" is simply to indicate that a mechanism's phenomenon depends not just on what the parts of the mechanism are, or on what activities those parts engage in, but on how the parts and their activities are arranged. Mechanisms are not just heaps of parts. To take a very simple example, the parts of an engine will not work as an engine unless the engine's parts are carefully arranged and connected. Similarly, the behavior of the animal's digestive mechanism depends upon how each of the parts is physically connected to each other, on the timing with which food passes through the system, on neural and endocrinological signals that impact the secretion of enzymes, etc. (2017, p. 23)

This suffices to clarify how we use the term 'mechanism' in this article. Let us now turn to 'mechanistic explanation'.

Mechanistic explanation

Because there are various types of mechanism for different types of phenomena, there are different types of mechanistic explanations. Since our explananda are regularities (see "Explanation-seeking questions" section) we only need a characterisation of what a mechanistic explanation of a regularity (abbreviated as MER) is. For or purposes, the following is adequate:

> [MER] A mechanistic explanation for a regular behaviour is an explanation in which the explanans is a description of the *type* of mechanism that produces the regular behaviour.

A description of a mechanism is usually called a model of the mechanism. Note that in [MER] the model of the mechanism is the explanans, which is only a part of the explanation. A mechanistic explanation also contains an explanatory derivation of the explanandum phenomenon from the model.

Mechanistic explanation of regularities: an example

Boyle's law states that for gases held at a fixed temperature and mass, the product of pressure (P) and volume (V) is constant ($P.V = k$, where k depends on the temperature and amount of gas). This law (and many other gas laws such as the more general ideal gas law)

can be explained by means of the kinetic model of gases (which fits into the general kinetic theory of matter; the overall theory also deals with properties of fluids and solids). As for entities, the most important tenets of the kinetic gas model are:

The system consists of gas molecules and a solid container.
The number of molecules is large.

The molecules exhibit a linear motion at constant speed, except during collisions. With respect to activities the crucial tenets are:

The molecules are in perpetual motion.
The walls of the container are rigid (so they do not move).
The molecules collide with each other and with the walls of the container.
These collisions are perfectly elastic (no loss of kinetic energy).

These tenets are approximately valid. The kinetic gas model describes 'ideal' gases. Crucial organizational tenets are:

The molecules are located within a (hermetically) closed container
The number of molecules moving in any one direction is, on average, the same as that moving in any other direction (i.e. the motion is on average random).

The explanation of Boyle's law by means of the kinetic gas model is mechanistic: the model describes entities, activities and organization. Explanatory derivations of Boyle's law from this model can be found in many physics and chemistry textbooks.

Physical dependency and why it matters for explanation

According to James Woodward (2003) explanatory derivations have to mirror physical dependency relations in order to be explanatory. This idea is presented in the "Physical dependency" section. In "Physical dependency and mechanisms" we show that mechanistic philosophers endorse the idea. All this material will be used in "Do quantum mechanical atom models (electronic configurations) provide legitimate explanations?" to address our first philosophical question.

Physical dependency

Woodward uses the criterion of *mirroring physical dependency relations* to distinguish explanatory derivations from non-explanatory derivations:

> The idea is that these derivations trace or mirror the relations of physical dependency that hold between the explanans conditions and the explananda phenomena – relations that would be revealed if, for example, we were to physically intervene to alter the explanans conditions. (2003, p. 201)

To illustrate what he has in mind, we compare two derivations:

For all flagpoles: $L = H / \tan \alpha$ (= Flagpole Law A).
The angle of elevation of the sun is 45°
This flagpole has a height of 10 m.
———————
This flagpole has a shadow that is 10 m long.

In the first premise, H stands for the height of the flagpole, L for the length of the shadow and α for the angle of elevation of the sun above the horizon. Compare this with the reversed derivation:

For all flagpoles: $H = \tan \alpha \times L$. (= Flagpole Law B).
The angle of elevation of the sun is 45°
This flagpole has a shadow that is 10 m long.
———————
This flagpole has a height of 10 m.

The first derivation is explanatory (according to Woodward) because it mirrors physical dependency relations. The second is not explanatory: the height of the flagpole does not physically depend on the angle of elevation of the sun nor on the length of the shadow. And despite the fact that Flagpole Laws A and B are mathematically equivalent, only A is an explanatory generalisation because it has the causes on one side of the equation (in casu: the right-hand side) and the effect on the other side.

The physical dependency requirement is connected to Woodward's view on explanatory power. The core idea is that "explanation is a matter of exhibiting systematic patterns of counterfactual dependence" (2003, p. 191). According to Woodward, a good explanation must also tell us how the explanandum would change if the initial conditions would be different. In other words, adequate explanations …

> … locate their explananda within a space of alternative possibilities and show us how which of these alternatives is realized systematically depends on the conditions cited in the explanans. They do this by enabling us to see how, if these initial conditions had been different or had changed in various ways, various of these alternatives would have been realized instead (2003, p. 191).

In the flagpole case, the explanation answers questions such as 'what would happen if the flagpole was 5 m high?' or 'what would happen if the sun was at 60° above the horizon?'. Woodward calls the counterfactual questions 'what-if-things-had-been-different' questions.

The connection between the counterfactual questions and physical dependency is that derivations that do not mirror a physical dependency (and hence are not explanatory) do not allow us to answer 'what-if-things-had-been-different' questions. In the flagpole example, the non-explanatory reversed derivation does *not* provide an answer to the question 'what would happen to the height of the length of the flagpole if the shadow was made shorter?' (e.g. by means of an additional light beam).

Physical dependency and mechanisms

Mechanistic philosophers endorse Woodward's idea of physical dependency. For instance, Stuart Glennan sees it as a sine qua non for explanation (2017, p. 212). This has implications for how certain key terms of mechanistic philosophy have to be understood. Let us have

a second look at the definition we gave in the "Mechanisms and mechanistic explanation" section:

> A mechanism for a phenomenon consists of entities (or parts) whose activities and interactions are organized so as to be responsible for the phenomenon. (Glennan & Illari 2018, p. 2)

The term 'responsible for' must be read as involving bottom-up determination, the behaviour of the whole physically depends on the activities of the entities and their organisation. This idea is visible in the use of alternative terms such as 'produce' or 'give rise to'. In some cases top-down derivations are possible. For instance, if my lawn mower mows the lawn as desired and expected, I can derive that certain components are present and that they perform certain activities. But the presence of the components and their behaviour is not physically determined by the higher level phenomenon. For instance, if I lift my lawn mower 20 cm above the ground (and hence ensure that it does not cut any grass anymore) this has no effect on the presence of the components and their activities.

Do quantum mechanical atom models (electronic configurations) provide legitimate explanations?

Introduction

The claims at stake in this section are:

> Quantum mechanical models of atoms provide legitimate explanations of physico-chemical behaviour regularities.
> Quantum mechanical models of atoms provide legitimate explanations of periodic table regularities.

The starting point is that the regularities (explanandum) can be derived from the electron configurations. The question is: are these derivations explanatory? For the physico-chemical behaviour regularities we give a positive answer based in the notion of physical dependency ("Legitimate explanations I: physico-chemical regularities" section). Our answer for the periodic table regularities is also positive (see "Legitimate explanations II: periodic table regularities"), but that uses an extra ingredient: the idea of unification, which we introduce in the "Unification as additional virtue" section.

Legitimate explanations I: physico-chemical regularities

In this section we argue that there is a 'bottom-up' determination in the quantum mechanical accounts of the physico-chemical behaviour regularities which is similar to what we mentioned in sect. 5.4. We focus on the first specific regularity mentioned in the "Explanation-seeking questions" section:

> Why is lithium a good electrical conductor?

In order to interpret this explanandum regularity properly, it should be stressed that conductivity is a macro-level property. A single atom cannot be conductive. We need an object (wire, bar, ball, lump, …) made up of many atoms (of lithium in this case), or a volume

of them contained in a vat (e.g. if the element is gaseous under natural conditions). Hence 'lithium' is to be interpreted here as shorthand for 'objects consisting of lithium atoms'.

The explanation which addresses this question consists of a model and a derivation (like the mechanistic explanations of Boyle's law discussed in "Mechanistic explanation of regularities: an example"). The core of the model is this:

Lithium atoms have two electrons in the *s*-shaped orbital of energy level 1.
Lithium atoms have one electron in the *s*-shaped orbital of energy level 2.
Lithium atoms have no electrons in the 2p orbital or at higher energy levels.

The core of the derivation is:

Initial condition
Lithium atoms in ground state have a single electron in the highest energy level.
Explanatory generalization 1
Atoms tend to donate, receive, or share electrons to realize a stable electronic configuration (i.e. the configuration of the nearest noble gas[2]).
Derived generalization 1
Atoms with full shell(s) and a single electron in the subsequent highest energy level (s^1) display a high tendency of donating said electron (leading to the electronic configuration of the previous noble gas).
Mediating condition
Lithium atoms have a high tendency of donating their outmost electron.
Explanatory generalisation 2
Objects in solid state consisting of atoms that have a high tendency to donate electrons are good electrical conductors. Objects consisting of atoms that have a high tendency to receive or to share electrons are good insulators. Objects consisting of atoms that have a slight tendency to donate electrons are semiconductors.

Explanandum regularity
Lithium is a good electrical conductor.

This derivation has two stages and involves two levels. First, a property of individual lithium atoms (the mediating condition) is derived from the internal structure of these atoms (the initial condition) by means of an overarching and a specific generalisation (the latter specifies wat the first entails when applied to the case at hand). Second, the explanandum regularity is derived from the mediating condition and a second explanatory generalisation which connects properties of individual atoms to a property of objects composed of them.

The initial condition describes a more abstract property of lithium atoms that is entailed by the specific properties described in the model. It identifies the relevant feature. This comparable to the kind of abstraction that Michael Strevens draws attention to (2008, p. 96–97). Suppose that I throw a 10 kg cannonball at a window and the window breaks. The fact that the cannonball is quite heavy is important for explaining that the window breaks. That its mass is exactly 10 kg is not important. Hence, the explanatory derivation can have a more abstract initial condition, e.g. 'The cannonball weighs more than 5 kg'.

[2] We assume the electronic configuration of noble gases is stable. This can also be further fleshed out in terms of lower energetic requirements, or made in to an explanandum which could require a different type of explanation, for example showing how s orbitals are symmetrical or showing that full shells shield the following orbitals from the nucleus.

The second generalisation follows from the Electron Sea Model (in the case of metals) or the Energy Band Theory (in the case of insulators and semiconductors). In the case of metals, 'donated' electrons are free to flow around the metallic structure, effecting an electrical current.

The crucial issue is whether the generalisations trace a physical dependency relations (and hence really is 'explanatory'). In our view the answer is positive because the generalisations allow us to answer counterfactual questions, such as 'what would happen if you consider helium atoms instead of lithium atoms?' In such a case, there is no tendency to donate electrons. From Explanatory generalisation 1 we can also derive:

Derived generalisation 2
Atoms in which the highest energy level is full have no tendency to donate electrons.

So helium is not a good electrical conductor. A similar argument could be applied to hydrogen, since it favours 'sharing' an electron rather than donating[3] it. Hydrogen is missing one electron to fill its first shell, leading to the electronic configuration of helium; hence it will not make a good electric conductor. This is an implication of another generalisation that can be derived from Explanatory generalisation 1:

Derived generalisation 3
Atoms missing one electron to complete their highest energy level have a high tendency to receive or share an electron.

Finally, questions such as 'what would happen if you consider sodium atoms instead of lithium atoms?' can also be answered: they would also be good electrical conductors (Derived generalisation 1 is used here).

Unification as additional virtue

As we mentioned before, Glennan sees (physical) dependency as a sine qua non for explanations. But it is not the only virtue that explanations can display. There is also unification:

> Explanatory models may show that two or more things are similar, either in what they depend upon, or in what depends upon them. (2017, p. 212)

Glennan sees unification as a desirable but non-essential feature. In this section we apply this idea to the QM models. We have argued that they explain certain physico-chemical behaviour regularities, because they establish a physical dependency. Now we will investigate whether there is something extra to be found: unification. Our answer is affirmative: the quantum mechanical models can be used to answer certain *resemblance questions*. In doing so, they provide unification.

What are resemblance questions? Explanation-seeking questions about regularities come in three types: plain questions, contrastive questions and resemblance questions. Examples of plain questions are:

Why do children of blue-eyed parents always have blue eyes?
Why are all ravens black?

Examples of contrastive questions are:

[3] Losing an electron leads simply to a proton, which given its high charge density will rapidly hydrate. In other words, losing an electron does not lead to a stable electronic configuration for hydrogen.

Why do pigeons have the capacity to find their way back home, while other sedentary birds do not have that capacity?
Why do woodcocks migrate during the night, while pigeons cover long distances during the day?

Examples of resemblance questions are:

Why do humans as well as desk calculators have the capacity to perform exact numerical calculations?
Why are ravens as well as crows black?

Note that all these questions, since they are questions about regularities, presuppose some kind of resemblance: ravens are similar in that they are black, woodcocks are similar in that they migrate at night. The three types of questions represent three possible directions in which attempts to understand the regularity can go. We can zoom in on the regularity itself (plain question), we can focus on differences with other regularities (contrastive question) or we can focus on similarities with other regularities (resemblance question). In the latter case we investigate a 'higher order resemblance': a resemblance between two regularities describing regular behaviour (i.e. resemblances in the behaviour of a class of systems).

Legitimate explanations II: periodic table regularities

In "Explanation-seeking questions" we mentioned three explanation-seeking question arising from periodic table regularities:

Why are alkali-metals in solid state good electrical conductors?
Why do halogens easily form compounds with alkali-metals?
Why do noble gases not form compounds under natural conditions?

These questions can be seen as resemblance questions of the following form:

Why do objects of class X as well as objects of class Y, Z, … have the capacity E?

Let us illustrate this by means of the first question. It can be reformulated as follows:

Why are lithium, sodium, potassium, rubidium, caesium, and francium good electrical conductors?
In this formulation, it becomes clear that there is a higher order resemblance that we can try to explain: a resemblance between several regularities each describing regular behaviour of a class of systems.

The explanation which addresses this question consists of a set of models (instead of one model as the explanations in "Legitimate explanations I: physico-chemical regularities") and a derivation. The models in the set are as follows:

(Li) The electron configuration of lithium atoms in ground state is $[He]2s^1$.
(Na) The electron configuration of sodium atoms in ground state is $[Ne]3s^1$.
(K) The electron configuration of potassium atoms in ground state is $[Ar]4s^1$.
(Rb) The electron configuration of rubidium atoms in ground state is $[Kr]5s^1$.
(Cs) The electron configuration of caesium atoms in ground state is $[Xe]6s^1$.
(Fr) The electron configuration of francium atoms in ground state is $[Rn]7s^1$.

The core of the explanatory derivation is:

Initial condition (explanans similarity)
In ground state lithium, sodium, potassium, rubidium, caesium, and francium atoms have a single electron in the highest energy level.
Explanatory generalization 1
Atoms tend to donate, receive, or share electrons to realize a stable electronic configuration (i.e. the configuration of the nearest noble gas).
Derived generalization 1
Atoms with full shell(s) and a single electron in the subsequent highest energy level (s^1) display a high tendency of donating said electron (leading to the electronic configuration of the previous noble gas).
Mediating similarity
Lithium, sodium, potassium, rubidium, caesium, and francium atoms have a high tendency of donating their outermost electron.
Explanatory generalisation 2
Objects in solid state consisting of atoms that have a high tendency to donate electrons are good electrical conductors. Objects consisting of atoms that have a high tendency to receive or to share electrons are good insulators. Objects consisting of atoms that have a slight tendency to donate electrons are semiconductors.

Explanandum similarity
Lithium, sodium, potassium, rubidium, caesium, and francium are good electrical conductors.

This derivation is genuinely explanatory because the generalisations trace physical dependency relations (see above). An example of a counterfactual question that is answered by it is 'what would happen if you consider helium atoms instead of lithium atoms?' The answer is that we would have a 'mediating contrast' (instead of a mediating similarity) and a 'final contrast':

Mediating contrast
While atoms in group 1 have a high tendency of donating electrons, helium atoms have no such tendency (they are already electronically stable).
Final contrast
While elements in group 1 are good electrical conductors, helium is an electrical insulator.

Summary and preview

We have argued for the following theses:

Quantum mechanical models of atoms provide legitimate explanations of physicochemical behaviour regularities.
Quantum mechanical models of atoms provide legitimate explanations of periodic table regularities.

Because we accept these theses, the answer to the first philosophical question is positive: atomic models of quantum mechanics do provide legitimate explanations. The next philosophical question is: are these explanations mechanistic? In this section we have shown that quantum mechanical explanations have some properties of mechanistic explanations: they

are ‘bottom-up’ explanations and the derivations mirror physical dependency relations. But that does not entail that they are mechanistic explanations: other properties of mechanistic explanations may be missing. This will be explored in the “Quantum mechanical models do not provide mechanistic explanations” section , which constitutes a second part of our comparison with mechanistic explanations: until now we have focused on similarities, from now on we investigate differences.

Quantum mechanical models do not provide mechanistic explanations

Introduction

Let us define ‘bottom-up explanations’ as explanations that invoke entities at a lower level compared to the level at which the explanandum phenomenon is situated. The quantum mechanical accounts are clearly bottom-up explanations in this sense: they involve decomposing atoms into nuclei and electrons, and thus invoke entities at a lower level.

We will argue that the quantum mechanical explanations, despite being bottom-up explanations (a feature they share with mechanistic explanations) are not mechanistic. The reason is that they do not provide the right kind of information. An argument against characterising the quantum mechanical accounts as mechanistic explanations can be built by further developing the classification of mechanisms and mechanistic explanations developed by Meinard Kuhlman and Stuart Glennan in the paper ‘On the Relation between Quantum Mechanical and Neo-mechanistic Ontologies and Explanatory Strategies’. We present this classification in the “Kuhlman and Glennan on classical and non-classical mechanisms” section. The most important insight of Kuhlmann & Glennan (for our argument) is that ‘non-classical’ mechanisms are possible in the quantum domain. In “Two Epistemological Clashes" we argue that, although non-classical mechanisms may exist in the quantum domain, the accounts presented in “Potential explanations for chemical regularities: quantum mechanical atom models” are not descriptions of such mechanisms. They describe systems in a non-mechanistic way: from a mechanistic perspective, they provide the wrong kind of information. Hence, they cannot be the starting point of mechanistic explanations.

Kuhlman and Glennan on classical and non-classical mechanisms

Kuhlman and Glennan distinguish four important features of neo-mechanistic ontology. The first important feature is that mechanisms consist of discrete parts and that the “parts are taken to be real things as opposed to explanatory constructs” (p. 339). The idea is that, if you decompose a mechanism into entities, “these decompositions are explanatory because they refer to real features of the world” (p. 339).

The second feature pertains to causality:

> A second feature of the New Mechanist consensus is the idea that phenomena exhibited by the mechanisms are *produced* by the *activities* and *interactions* of parts. The terms ‘activity’, ‘interaction’, and ‘produce’ are all transparently causal. If the activities and interactions are not genuinely causal, then mechanism can’t produce anything. Mechanistic explanation is a species of causal explanation and the legitimacy

> of mechanistic explanation depends upon the interactions between parts being genuinely causal. (2014, p. 339; italics in original)

The third feature is the focus on organisation:

> It is the organization of the entities (and their activities) that allows the mechanism to produce the phenomenon that it does. A pile of lawnmower parts does not [make] a lawnmower. While mechanists emphasize the importance of spatial and temporal organization, it is ultimately the causal organization upon which the productive capacities of the mechanism depend. (2014, pp. 340-341)

The fourth feature is the focus on the hierarchical organisation of mechanisms: mechanisms and the phenomena they produce may in turn be embedded in larger mechanisms (2014, p. 341).

Kuhlmann & Glennan identify three potential clashes between neo-mechanistic ontology and quantum ontology: indeterminacy of properties, non-localizability of quantum objects and non-separability of quantum states due to entanglement. We do not discuss this in detail, because we think they have convincingly argued that these are only prima facie clashes. In their discussion of the second potential clash they develop a classification of mechanistic systems and mechanistic explanations that is useful for our argument. They introduce the idea of 'non-classical mechanisms' which they distinguish from two other classes of mechanisms that are 'classical'. The latter are described in the following quote:

> We shall argue that localizability of parts, while important in many classical mechanistic explanations, is not an indispensable feature of mechanistic explanation. The reason is that the fundamental mode of organization that matters in mechanisms is causal dependence, not spatial location. It is only when spatial location determines causal dependence that spatial location is essential to mechanistic explanation. In some mechanistic systems spatial location is absolutely essential. For instance, in the lawn mower discussed in Section 2, the capacities of the various parts to interact with each other depend upon them being physically situated in exactly the right way. But in other thoroughly classical systems this is not the case. Consider for instance a system consisting of an ensemble of radio transmitters and receivers. Whether a particular receiver is connected to a particular transmitter will not depend upon its specific location, but upon whether it is tuned to receive the transmitted frequency. (2014, p. 354).

For our purposes it is good two have a concise and precise characterisation of the two classes:

> *Class 1 mechanistic models*
> Models like the description of the lawn mower in which a strict spatial organisation is posited and this organisation is claimed to determine causal relations.
> *Class 2 mechanistic models*
> Models like the transmitter/receiver model in which the spatial organisation is not specified (even though it would be possible) because it is considered irrelevant: this organisation does not determine causal relations. The model does describe the causal organisation of the system.

Kuhlman & Glennan oppose these two classes to a third class of mechanisms and mechanistic explanations, which is described as follows:

> In conclusion, we think it is appropriate to say that the behavior of a composite quantum system is, under circumstances like those of the laser, due to what we call a "non-classical mechanism": The mechanistic explanation shows how a stable behavior of a compound system reliably arises purely on the basis of the interaction of its constituents, where it is the causal organization that matters and the spatiotemporal organization remains almost completely unspecified. One important difference between this case and our case of the classical set of transmitters and receivers is that in the classical case, it is possible to attribute locations to the parts while in the non-classical case it is not. But whether classical or non-classical, spatial organization is in both cases irrelevant to the mechanistic explanation. (2014, p. 356)

To facilitate our argument, we again give a concise and precise characterisation:

> *Class 3 mechanistic models (non-classical)*
> Models like the quantum mechanical model of the laser in which no spatial organisation is given because it is impossible to specify it. Luckily, this organisation does not determine causal relations. The model does describe the causal organisation of the system.

The most important difference between class 2 and class 3 models is that in class 2 you leave out spatiotemporal details for reasons of efficiency. In class 3 you leave them out because you have no choice. You cannot include them, but you still have an explanation because you can describe the causal organisation.

Two epistemological clashes

The quantum mechanical explanations invoke entities at a lower level: they involve decomposing atoms into nuclei and electrons. These elements have a strict, orderly organisation: the characteristic electron configuration of each type of atom. Nevertheless, the quantum mechanical models do not provide the right kind of information in order to function as explanans in mechanistic explanations. Atoms may be mechanistic systems (there may be activities and causal influences) but the quantum mechanical accounts (focusing on electronic configuration) are not models of mechanisms. They describe *other features* of the systems. More specifically, it is the case that:

> (a) The quantum mechanical models of atoms detail permanent properties of atoms but remain silent about activities (in the mechanistic sense).
> (b) The quantum mechanical models of atoms detail spatial organisation but remain silent about causal organisation.

Let us discuss both divergences in detail.

'Occupying an orbital' is a feature of an electron but it is debatable whether it is an activity. An activity is something that starts at some point in time and ends at a later point in time. Furthermore, by definition, an activity requires action; occupying space does not constitute any form of action. The quantum mechanical models discussed in this paper describe the permanent structure of a class of systems. They do not provide information about activities or processes that sometimes go on in the systems. Hence, they cannot provide mechanistic explanations: they do not give the right kind of information. Note that this is not an ontological clash: there may be activities in atoms, but the models do not describe them.

There is also a divergence with respect to causal organisation. The issue is that no information about causal organisation is described in the present quantum mechanical models. To clarify this, we contrast it with the lawn mower:

> To clarify the role or organization in mechanisms, consider as a brief example the mechanism for starting a lawnmower engine. The engine is started by rapidly pulling a cord while the throttle is set to an appropriate level. The cord is attached to a flywheel which in turn engages a clutch which causes the crank shaft to move, which in turn moves the piston, allowing air and fuel into the cylinder. The flywheel is also connected to a magneto—a device which uses the rotation of magnets to generate a voltage. The magneto is attached to the sparkplug which produces the spark that ignites the fuel-air mixture in the piston. The production of the phenomenon (namely the starting of the mower) *depends essentially on organization*. The parts must be spatially organized so that the same part—the flywheel—may simultaneously engage the clutch and turn the magneto. Timing is also essential here. The parts must be so organized that the spark generated by the spark plug enters the cylinder at the correct time in the piston's cycle. *These spatial and temporal arrangements determine the causal organization of the system*. (2014, p. 341; emphasis added)

Even though the chemical elements have a strict, orderly organization (viz. the characteristic electron configuration of each type of atom) this is not a 'causal organization'. The spatial organization is *not connected* to any causal interaction that there may be between the electrons. For instance, it is certainly not the case that only electrons within the same orbital can have an influence on each other's behaviour. Again, we are not claiming that electrons do not as a matter of fact have causal influences on each other. We claim that these influences are not depicted by the electronic configuration of each atom.

Lessons

Let us take stock. In "Do quantum mechanical atom models (electronic configurations) provide legitimate explanations?" we have argued for a positive answer to our first philosophical question:

> Do quantum mechanical models of atoms provide legitimate explanations?

This positive answer generated the second philosophical question:

> Are the explanations provided by quantum mechanical models of atoms mechanistic explanations?

In this section we have argued for a negative answer to this question. The explanations are not mechanistic because the models belong to a fourth class:

> *Class 4 models (non-mechanistic)*
> Models (such as the quantum mechanical atom models above) in which the spatial organisation is specified but does not refer to causal relations between active and interacting parts. The causal organisation of the system is not described. The model also remains silent about (mechanistic) activities, although it describes permanent properties.

Our positive answer to the first question, combined with the negative answer to the second question, raises a third philosophical question:

What kind of explanation do quantum mechanical models of atoms provide?

This question is addressed in the "Structural explanations and structural unification" section .

Structural explanations and structural unification

Structural explanations

Our first move in answering the third question is to give a label to the type of explanations that we find in the quantum mechanical accounts of physico-chemical behaviour regularities. We call them structural explanations. This term has been used by many philosophers of explanation. Some use it as an umbrella term for all explanations that are not clearly causal or mechanistic, and hence a bit strange or peculiar (e.g. Glennan 2017, p. 237). Other philosophers use it in a more specific sense. That is also what we do. Our definition is:

> An explanation is structural if and only if (i) the explanandum physically depends on the micro-structure described in the explanans and (ii) the explanans is a class 4 model.

By means of this definition, a partial answer to the third question can be given:

> Quantum mechanical models of atoms provide structural explanations for physico-chemical behaviour regularities.

To obtain a complete answer, we introduce the concept of structural unification.

Structural unification

We define structural unification as follows:

> Structural unification consists in the act of answering a resemblance question by identifying a crucial common feature (explanans similarity) in a set of micro-structures, where (i) the models that describe these micro-structures are class 4 models, and (ii) each element of the explanandum similarity physically depends on the corresponding micro-structure.

In the example in "Legitimate explanations II: periodic table regularities", the crucial common feature is that all the elements find it energetically favourable to lose the single electron in their highest energy level. Structural unification as defined above fits into Glennan's characterisation ("Unification as additional virtue" section): it allows us to see that apparently disconnected phenomena are connected, because there is a similarity in the micro-structures that produces them.

By means of this definition, the second half of our answer to the third question can be given:

> Quantum mechanical models of atoms provide structural unification with respect to the resemblances underlying the periodic table regularities.

Comparison with mechanism unification

In earlier work (Weber & Lefevere 2017) we introduced the idea of mechanism unification. Like structural unification, mechanism unification addresses resemblance questions about regularities. The format of these questions is:

> What are the common features of the mechanisms that produce capacity E in objects of type X, Y, Z, …. ?

An example of such question is:

> What are the common features of the mechanisms that produce the capacity to perform exact numerical calculation in humans and in desk calculators?

Our 2017 paper contains an elaborate case study on anaesthesia and its history. Many chemical substances can induce general anaesthesia (i.e. they simultaneously cause unconsciousness, amnesia, analgesia, and muscle relaxation). This leads to the following resemblance question:

> What do the mechanisms by which the chemical substances X, Y and Z induce general anaesthesia have in common?

The act of mechanism unification consists in providing the richest possible mechanistic model that is correct for objects of type X as well as objects of type Y and Z. Mechanism unification in this sense produces the most informative correct answer to questions of the type above. It results in explanations that are both mechanistic *and* unifying.

Mechanism unification allows us to see that apparently disconnected phenomena are connected: there is a similarity in the mechanism that produces them. Like structural unification, it fits into Glennan's characterisation of unification.

Some comparisons

Lauren ross

As we have seen in the introduction, Lauren Ross argues that scientists frequently appeal to atomic structure when explaining the chemical and physical properties of elements. This raises several philosophical questions:

> If electronic and atomic structure play a role in explaining the periodic behavior of the elements, how should we understand these explanations? What role does the periodic table play in this explanatory process and is it best understood as causal in nature? (2021, p. 84)

Let us see what our answers to these questions are and how they relate to the views of Ross. In "Structural unification" we have argued that the explanations should be conceived as providing structural unification. That is our answers to Ross' first question.

Our analysis 6.4 sheds light on the role of the periodic table in the explanations: it provides the information that goes into the initial condition of the explanation. In our analysis, the periodic table is a handy source of information about explanans similarities. To see why this is important, let us look back at the flagpole example in the "Physical dependency" section. The explanation requires descriptive information

we obtain by means of measurements of the height of the flagpole and the position of the sun. And it also requires general knowledge about causal dependence between the variables. Similarly, the explanation in "Legitimate explanations I: physico-chemical regularities" requires descriptive information (the explanans similarities) and knowledge that establishes physical dependencies. The descriptive information comes from the periodic table (as opposed to specific measurements as in the flagpole case) while the knowledge that establishes physical dependence comes from theoretical chemistry (Electron Sea Model, Energy Band Theory, …). In sum: our view is that scientists invoke the periodic table to introduce initial conditions.

Eric Scerri has claimed that "the periodic table is only a chart or a graphical classification rather than any form of deep explanation." (2020, section 6). We would go a step further: the periodic table in itself has no explanatory power at all, because it is just handy systematic summary of potential initial conditions of explanations. In order to have an explanation, a lot of knowledge that originates in theoretical chemistry has to be connected to these initial conditions. The periodic table is a chart that provides one type of information that goes in to the explanation. The other type of knowledge that we need is not present in the table.

A corollary of this is that the periodic table is best viewed as non-causal in nature: it is a description of similarities and differences that (when combined with theoretical chemistry) are useful for explaining other similarities and differences.

Andrea Woody

Andrea Woody observes what she takes to be a puzzle. On the one hand, scientists connect the periodic table to explanation. On the other hand …

> … the periodic table seems a rather poor candidate for explanatory status under any of the traditional philosophical accounts of scientific explanation. There is no explicit logical statement of the law; it does not reveal causal structure, identify mechanisms, serve as premises in articulated argument patterns, or in any obvious manner aid the attainment of empirical adequacy. Rather, the table is valuable because of its ability to reveal, or make perspicuous, certain relations. (2014, p. 143)

Our view is that there is no tension, because the table can provide valuable information that goes into explanations without having 'explanatory status' in itself. The information derived from the table can even be indispensable for constructing the explanation, but our view is that the table should not be looked at in isolation when you are investigating its explanatory value. Invoking the table in an explanation together with a good deal of theoretical chemistry is not the same as saying that the table can provide explanations all by itself. So we are happy with what the situation that Woody describes:

> Although many will agree that the periodic table organizes, and even classifies, there is no similarly robust intuition that it explains. (2014, p. 141)

The table indeed organises and classifies, and this information can become part of an explanation. But the table in itself does not explain.

Conclusions

By addressing our three philosophical questions, we have tried to shed light on an important type of chemical explanation. Our investigation resulted in five theses:

1. Quantum mechanical models of atoms provide legitimate explanations of physico-chemical behaviour regularities.
2. Quantum mechanical models of atoms provide legitimate explanations of periodic table regularities.
3. The explanations provided by quantum mechanical atom models are not mechanistic.
4. Quantum mechanical models of atoms provide structural explanations for the physico-chemical behaviour regularities.
5. Quantum mechanical models provide structural unification with respect to the resemblances underlying the periodic table regularities.

These results are important for philosophy of chemistry, but also for general philosophy of explanation. Scientific explanation comes in many forms, and our results increase our insights into what kinds of explanations exits and how they relate to each other.

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