Where do theories come from?

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What is the origin of spectacular new theoretical insight? What preconceptions enter into our models of the world and how strong are they influencing our way of thinking? Can we really probe into a platonic realm of universal ideas or do theories gain support more by creating shared belief? And to what extend can we benefit from conceptions outside the field of natural sciences? I want to approach such questions on the basis of examples from mathematics, physics, and chemistry, gaining some insight into the inner structure of theories.

1 Weyl's purely infinitesimal geometry

The first example points towards motivations for developments in mathematical geometry that come from a field of pure philosophy. The question about the origin of space was answered by Kant as being an *a priori* intuition that makes references to outer sensations possible in the first place. It is such not derived from experience because experience itself relies on it to organise perceptions. This already transcended the absolute space of Descartes and Newton and opened the way for synthetic concepts. Later Fichte, though never arguing genuinely mathematically, shifts the given idealities of space and time to those of material objects and argues for an emergence of the former. This led to the early realization that "time and space [...] are intimately interlinked" and that "time can only form itself in space."[1] It is not hard to imagine that such eminent philosophers writing about basic geometrical conceptions would influence the mathematics of the time. Bernhard Riemann in his habilitation talk in 1854 that presented possible generalizations of Euclidean space to n-dimensional and curved spaces also questioned the established absolute concept:

> It is known that geometry assumes, as things given, both the notion of space and the first principles of constructions in space. She gives definitions of them which are merely nominal, while the true determinations appear in the form of axioms. The relation of these assumptions remains consequently in darkness; we neither perceive whether and how far their connection is necessary, nor a priori, whether it is possible.

Hermann Weyl besides his significant contributions to mathematics and theoretical physics had a strong interest in philosophy, especially in Husserl and Fichte.[2] This lead

[1] As cited by David M. Wood, *"Mathesis of the Mind" – A Study of Fichte's Wissenschaftslehre and Geometry* (2012).

[2] The main reference for the whole section is Erhard Scholz, *Hermann Weyl's "Purely Infinitesimal Geometry"* (1995), see also Norman Sieroka, *Husserlian and Fichtean Learnings: Weyl on Logicism,*

him to challenge the then newly constructed logical framework of 'classical' mathematics with axiomatic set theory at its core, a pursuit most prominently featured in his book *The Continuum*. This happened in the turmoil of the foundational crisis of mathematics sparked by Cantor that reached its peak in the 1920ies.[3] By then several new schools of mathematics had formed. One of them, advocated by Poincaré and for some while by Weyl, is predicative mathematics, abandoning all implicit definitions including the object being defined and thus avoiding the vicious circle of Russell's paradox. A more radical school is constructive mathematics like Brouwer's intuitionism to which Weyl was won over later. In constructivism a truth value means "a proof can be given", so what can be said about a statement like "every even integer > 2 is the sum of two primes"? Up to date Goldbach's conjecture is unresolved and following Gödel's incompleteness it might always remain, so in constructivism it is neither true nor false. Thus the general validity of the law of the excluded middle is refused and a proof by contradiction becomes void. Such deep scepticism had to permeate all fields of mathematics and in his thoughts about the continuum Weyl was criticizing the set-theoretic approach that

> contradicts the essence of the continuum, which by its very nature cannot be battered into a set of separate elements. Not the relationship of an element to a set, but that of a part to the whole should serve as the basis for an analysis of the continuum.[4]

To make that "relationship of a part to the whole" manifest he needed to address the issue of measurement of length in Riemannian manifolds, whose inventor wrote for his habilitation talk that

> measure-determinations require that quantity should be independent of position, which may happen in various ways. The hypothesis which first presents itself, and which I shall here develop, is that according to which the length of lines is independent of their position, and consequently every line is measurable by means of every other.

But the usual notion of length in Riemannian manifolds involves an absolute scale, only direction is taken to be relative to the position. Weyl's view on the continuum urged him to keep meaningful relations only in infinitesimal neighbourhoods of points, thus denying the possibility to directly compare the length of two tangent vectors $\xi \in T_pM$ and $\eta \in T_qM$ if $p \neq q$. This led to the proposal of a relative length scale attached to every point of the manifold, arriving at the structure of a (trivial) fibre bundle $M \times \mathbb{R}_{>0}$, and

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Intuitionism, and Formalism (2009) for claims of influences from philosophy on Weyl.

[3] In 1928–29 Hilbert kicked Brouwer from the board of *Mathematische Annalen* in a quarrel that also affected Einstein and Carathéodory and ended Brouwer's professional career, see `http://plato.stanford.edu/entries/brouwer`.

[4] As cited by Scholz from Weyl's *Riemanns geometrische Ideen, ihre Auswirkungen und ihre Verknüpfung mit der Gruppentheorie*.

a corresponding transfer principle between infinitesimally close points analogous to Levi-Civita's connection for directions. Scholz expresses that in this way "relations between quantities in different neighborhoods (of finite distance) ought to be considered meaningful only by mediation of the *whole*." Taking a parametrized curve γ such a length connection 1-form φ then gives the infinitesimal length calibration of a scale l at point $\gamma(0)$ in direction $\dot\gamma(0) \in T_{\gamma(0)}M$ as

$$(\partial_t l(\gamma(t)))\big|_{t=0} = -\varphi(\gamma(0))l(\gamma(0)).$$

This results in a generally path dependent length comparison. If one wants to contrast two different possible paths, one is lead to consider the two different routes along the edges of an infinitesimal parallelogram spanned by $\alpha, \beta \in T_pM$. The infinitesimal length difference of the two paths is the *length curvature* 2-form

$$f(\alpha,\beta) = \mathrm{d}\varphi(\alpha,\beta).$$

This new formalism was especially intriguing for Weyl because it reminds of the electromagnetic field f_{ij} and the associated 4-potential φ_i with the first set of Maxwell's equations being simply the exactness of f.

$$\mathrm{d}f = \mathrm{dd}\varphi = 0$$

A second set of source equations could now be added to make the analogy complete and to give a direct connection between electric charge and geometry. With this purely infinitesimal geometry gravitational and electromagnetic effects should be unified—gravity relating to the change of direction and electromagnetism from such length calibration—, contributing to a theory of dynamic matter creation proposed by Mie and Hilbert with particles as 'knots' coming from non-linear field equations with Lagrangians of the kind $L(g, Dg, D^2g, \varphi, D\varphi)$. This pursuit did not succeed but it nevertheless pioneered gauge theories and showed the fruitfulness of inspirations from philosophical considerations.

2 The principle of the conservation of energy

Ernst Mach in his book *History and Root of the Principle of the Conservation of Energy* (first published 1872), apparently the first historical account of its kind,[5] mentions the tremendous fruitfulness of the early principle that excludes perpetual motion without external causes in a time that had no concept of energy as it is known today. He identifies it as the logical root of the theorem of the conservation of energy, "considered as the flower of the mechanical view of the world, as the highest and most general theorem of natural science, to which the thought of many centuries has led." But already in the times of Galileo it was the presupposed basis for conclusions about the nature of forces though only formulated in an informal and very commonsensical way. The first example Mach gives in his book is from Stevinus' work *Hypomnemata mathematica*, Tom. IV, *De statica* of 1605, first published 1586.

[5]As noted by Ivan Illich in *The Social Construction of Energy* (1983).

A cord with attached identical turnable balls is slung around a triangle with differently tilted surfaces, four on the left and two on the right side. The cord below the triangle with additional balls is symmetrical and thus adds its weight equally to both sides. The distance between all the balls as seen from above is identical, thus the right surface of the triangle has double the inclination as the left one. Now one could suppose the eight balls on the left side dragging up the remaining six balls on the right side due to their greater weight. Stevinus, quoted by Mach, notes:

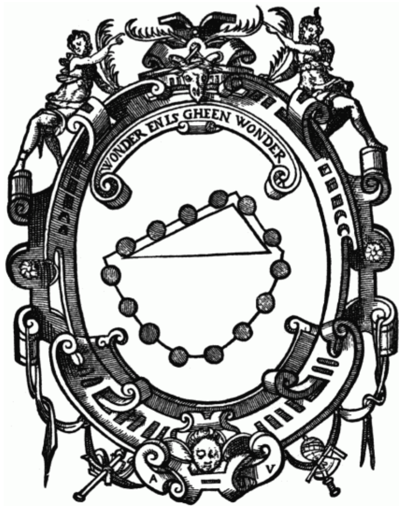

Figure 1: Cover page of *Hypomnemata mathematica* (taken from Wikipedia); the motto translates to "wonder is no wonder (at all)" meaning everything can be properly explained by science.

> But if this took place, our row or ring of balls would come once more into their original position, and from the same cause the eight globes to the left would again be heavier than the six to the right, and therefore those eight would sink a second time and these six rise, and all the globes would keep up, of them selves, *a continuous and unending motion, which is false.*

Thus by excluding such perpetual motion, *which is false*, he is able to conclude that the system has to remain in equilibrium and derives numerous fruitful consequences regarding the nature of forces. Now from a more modern viewpoint a continuing motion of constant speed may seem possible without friction but clearly not an accelerated one as would be the case with the balls on the left side always being heavier than those on the right side. But that does not change anything in the value of the conclusion, its truth in terms of mechanics, and the insight that a sentiment about the conservation of energy was already included even though it took more than 100 years for the notion of "energy" to arise and until the mid-1800s for it to arrive at its modern formulation. After Stevinus also Galileo and Huygens used the principle of excluded perpetual motion with great effect for mechanical problems and it was introduced to the domains of liquids and heat. Huygens reformulated it as a principle linking the height of ascent of the centre of mass of a body (like a pendulum) and the motion resulting from the effect of gravity. Such it became the foundation of a "law of the conservation of living force."[6]

But where does such a basic principle come from? And how could one be sure about its validity? Mach identifies its logical root in a very basic and early insight about causality

[6] The *vis viva* of Leibniz that later became kinetic energy.

and *not*, as one might think, as a theorem derived from basic mechanical laws of which it is ultimately a foundational piece. Mach draws on his contemporary Fechner in stating as a law of causality: “Everywhere and at all times, if the same circumstances occur again, the same consequence occurs again; if the same circumstances do not occur again, the same consequence does not.” Application of this rule directly shows up in Stevinus' quote when he refers to the “same cause”. But Mach argues against the dependency on the concepts of space and time, even to a much higher degree than Weyl after him. This view of Mach, also expressed in his famous argument against inertial frames detached from physical bodies, fully dismisses space and time as being fundamental. For example any measurement of time relies on a physical process serving as a clock.[7] By describing a phenomenon with respect to time, we just establish a law-like connection between two outer phenomena. Thus causality is reformulated as the very general “presupposition of the mutual dependence of phenomena.”[8] This tells us that between natural phenomena $\alpha_1, \dots \alpha_n$ equations of the form $f(\alpha_1, \dots \alpha_n) = \text{const.}$ can be set up that provide us with such law-like dependencies. The law of causality thus really stands at the very beginning of all exact science and simply proclaims *that a natural law can be stated.*[9] But any talk about laws directing the motions of everything in the universe is then superfluous because if all phenomena are included in a law, there is none left to serve as a clock, thus effectively freezing the full state of affairs. No inference from the known state of the universe to the next instant is thus conceivable. It is like Lewis Carroll's story of a map of scale 1:1 which is arguably very accurate but not of any practical use.

Now this basic conception of causality, the interrelatedness of perceptions, usually strikes us in childhood when one tries to grasp reason, cause, and effect of everything that surrounds us in a process called *learning*. So it seems no wonder that in the early days of mechanics it was already present. Let us derive a second similarly obvious law by considering a weighting scale with arms of equal length and equal weights on both sides, we must conclude—like Archimedes did before us—that it is in a state of equilibrium because there is simply no reason why it should turn in one direction rather than the other. We recognize such an application of the “law of sufficient reason” as complementary to the law of causality because now we have no phenomena at hand to which a specific outcome could be attached. If we paint the arms and weights of the scale in different colors we, scientifically educated, still expect the same outcome although now a phenomenon is perceivable. Mach gives his account to that peculiar ‘scientific’ reasoning: “Science has grown almost more by what it has learned to ignore than by what it has had to take into account.”

[7] Weyl in the introduction to *Space, Time, Matter* (1922) localizes this clock in the process of thinking, stating: “Time is the primitive form of the stream of consciousness.” This echoes Kant's words about time as a “pure form of the sensuous intuition.”

[8] Note especially that there is no ordering in time included in this formulation.

[9] This view was strongly supported by Ernst Mach's follower on the chair of natural philosophy in Vienna Moritz Schlick for whom causality is the *conditio sine qua non* of natural laws.

Returning to the concept of energy we imagine some phenomenon α (like the displacement out of equilibrium of a pendulum) to be the source of work if as an effect of this work performed, another phenomenon β (the bob's velocity) varies if α does. Any variation of β requires the same from α through a causal relation of the type $e(\alpha, \beta) = \text{const.}$ We have thus arrived at a statement of excluded perpetual motion of β in absence of an external cause α or—what seems even more—a law of the conservation of 'energy' e. This shows that this law, often stated as foundational for physics, is just an application of a very basic concept of causality and that energy is really just a universal link, including as many phenomena as possible in a relation that yields a scalar value. In this role energy is heavily used as the principal common denominator between different fields, bringing physical phenomena like motion, electricity, and heat together, acting like a currency, as a means of exchange, fundamental constants taking the role of exchange rates.[10]

If somebody shows you a machine, claiming it is a *perpetuum mobile* forever moving detached from all external sources of energy, the usual reaction will be the self-confident proclamation that there *must* be a *causal* explanation. So what happens is that in spirit of the exact sciences such an explanation in causal terms, i.e., a relation between external phenomena ξ and the *perpetuum mobile* π, written $f(\xi, \pi) = \text{const.}$, is sought for. If this quest leads to success by involving priorly unconsidered phenomena ξ, the machine is again integrated into the domain of reason and science; a *new* profound law of conserved quantities is found, extending the laws of nature. We might by convenience always call this most general conserved quantity the 'energy', methodologically reducing its law of conservation to a mere tautology.

John Stallo in *The Concepts and Theories of Modern Physics* (1888) agrees with this view on the principle of the conservation of energy: "In a general sense, this doctrine is coeval with the dawn of human intelligence. It is nothing more than an application of the simple principle that nothing can come from or to nothing." These words echo old Lucretius' "*res* [...] *non posse creari de nihilo, neque item genitas ad nil revocari*" and by describing the works of Epicurus this basic concept is put to work to deduce the conservation of both mass and motion. Epicurus' successors used it for the discovery of the neutrino (missing energy in the β^- decay) and the conjecture of dark energy (missing energy responsible for the accelerated expansion of the universe). In the next section different contributions to energy by the individual terms of a Hamiltonian will be set to work to explain the structure of molecules and such laying the foundations for the whole field of chemistry.

[10] In his text *The Social Construction of Energy* (1983) Ivan Illich gives an elaborated account on this analogy and links it to a "regime of scarcity" facilitated by modern science.

3 The conception of molecules in quantum chemistry

The generally accepted foundational law for all effects of chemistry is Schrödinger's equation. To fully account for bond and ionization energies its time-independent version is considered sufficient and all relevant information about the chemical structure is thought to be contained in the lowest eigenstate of the Hamiltonian. As this still poses a formidable problem one is bound to several layers of approximation, each one physically well founded of course, where the full molecular Hamiltonian is reduced to a form where calculations become numerically feasible. The ladder usually starts with the Born–Oppenheimer approximation requiring that the electron wavefunction is first treated with fixed values for the nuclear degrees of freedom (like vibrational and rotational modes).

$$E = E_{\mathrm{el}} + E_{\mathrm{vibr}} + E_{\mathrm{rot}}$$

This kind of summation of energies is clearly reminiscent of its use as a universal currency of different physical effects. The calculated electronic energy is then inserted into Schrödinger's equation dealing only with the nuclear wavefunction or combined with a classical treatment of nuclei. Already at this stage the nuclear geometry is designed after known structural formulae, a representation employed since the 1860ies.

Because the number of electronic degrees of freedom is still much too high in any space grid of reasonable resolution one has to further reduce them. This usually involves an expansion of the full electronic wavefunction into so-called molecular orbitals that account for covalent chemical bonds by encompassing multiple atoms. Those molecular orbitals come from linear combinations of a chosen basis set like the hydrogen orbitals where the coefficients are calculated with the Hartree–Fock method such that again minimal energy is achieved. A different and computationally less costly approach is Density Functional Theory (DFT) where the degrees of freedom are essentially reduced to the overall charge density. Needless to say, this involves further approximations.

DFT stems itself from the Hohenberg–Kohn theorem roughly stating that the charge density of a (non-degenerate) ground state uniquely fixes the effective external potential for interacting and also for fictitious non-interacting electrons. Thus in principle it is possible to substitute any system of interacting electrons with one of non-interacting electrons but with an added auxiliary potential that accommodates for all inter-electron effects. This new system is now much easier to solve because the single-electron Schrödinger equations decouple and the resulting orbitals can just be filled up one after another. That way a different electronic structure is produced but one still gets the same charge density by virtue of the Hohenberg–Kohn theorem. This serves as the remaining functional variable of all other properties of interest, particularly the energy, thus the name "Density Functional Theory". Such an approximation for the energy is applied to a further partition of the energy functional.

$$E_{\mathrm{el}} = E_{\mathrm{kin}} + E_{\mathrm{ext}} + E_{\mathrm{H}} + E_{\mathrm{xc}}$$

The kinetic energy and the energy of the electrons in any external potential are straightforward. The inter-electron effects are approximated by the Hartree term describing the mean Coulombic repulsion given by the charge density. All hope rests on the last term, the exchange-correlation energy, that needs to account for all quantum effects. Richard Feynman in his *Statistical Mechanics* (1972) notes that E_{xc} remaining without any idea for an exact expression is sometimes called "stupidity energy". It gets approximated by quite arcane methods, sometimes involving numerous parameters that are fitted to test scenarios or taken from experience. Dozens of different such "functionals" exist, each performing good for one type of problem (like metals, organics, different bond-types etc.) and worse for others. Yet this heavily approximative theory is most successfully applied, impressively displayed by Sidney Redner's *Citation Statistics From More Than a Century of Physical Review* (2004) where all three Top 3 most cited papers are from the field of DFT. The theory lies at the core of a whole industry of computer-aided chemical computation, enabling the calculation of properties of manually manipulated molecules. The product description of a popular software package called Gaussian/GaussView that also produced the figure below states:

> With GaussView, you can import or build the molecular structures that interest you, set up, launch, monitor and control Gaussian calculations, and retrieve and view the results, all without ever leaving the application. GaussView 5 includes many new features designed to make working with large systems of chemical interest convenient and straightforward. [...] We invite you to try the techniques described here with your own molecules.[11]

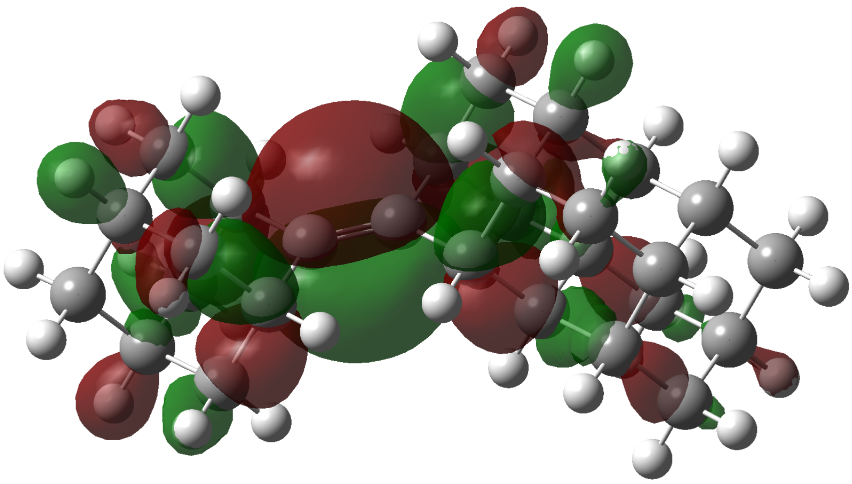

Figure 2: Adamantylidenetriamantane $C_{28}H_{36}$, the figure shows a 2% isoline of the highest occupied molecular orbital, variants of this chemical are used in various medical treatments (courtesy of Yusuf Mohammed)

[11] `http://www.gaussian.com/g_prod/gv5b.htm`

The long way from Schrödinger's equation to useful approximations casts the method far into the domain of phenomenological laws, those are laws that really connect to nature in that one gathers experimental evidence for them in practice. This is also the reason why Nancy Cartwright in *How the Laws of Physics Lie* (1983) attributes 'truth' only to such phenomenological laws, while the theoretical, fundamental laws like Schrödinger's serve as explanations and rules to guide our physical intuition. This split in the realm of scientific laws also finds expression in Hermann Weyl's writings:

> If phenomenal insight is referred to as knowledge, then the theoretical one is based on belief— the belief in the reality of the own I and that of others, or belief in reality of the external world, or belief in the reality of God. If the organ of the former is "seeing" in the widest sense, so the organ of theory is "creativity".[12]

"Science does not discover; rather it creates", writes Boaventura de Sousa Santos in *A Discourse on the Sciences* (1992). Such a science can be seen as an economical pursuit, a method to save thought and to provide laws as mnemonic tricks. But again this is no new conception at all and has been nicely expressed in the introduction of one of the classical masterpieces of science, Copernicus' *De revolutionibus orbium coelestium* (1543), in an unsigned letter by Andreas Osiander meant to calm down hostile reaction from the church, added without Copernicus' permission and sometimes viewed as a betrayal on the realist program of natural science. But it might tell something about where theories come from if they are not supposed to be divinely revealed to us.

> For it is the duty of an astronomer to compose the history of the celestial motions through careful and expert study. Then he must conceive and devise the causes of these motions or hypotheses about them. Since he cannot in any way attain to the true causes, he will adopt whatever suppositions enable the motions to be computed correctly from the principles of geometry for the future as well as for the past. The present author has performed both these duties excellently. For these hypotheses need not be true nor even probable. On the contrary, if they provide a calculus consistent with the observations, that alone is enough. [...] For this art, it is quite clear, is completely and absolutely ignorant of the causes of the apparent nonuniform motions. And if any causes are devised by the imagination, as indeed very many are, they are not put forward to convince anyone that are true, but merely to provide a reliable basis for computation. However, since different hypotheses are sometimes offered for one and the same motion (for example, eccentricity and an epicycle for the sun's motion), the astronomer will take as his first choice that hypothesis which is the easiest to grasp. The philosopher will perhaps rather seek the semblance of the truth. But neither of them will understand or state anything certain, unless it has been divinely revealed to him.

[12] Weyl (1925), from `http://plato.stanford.edu/entries/weyl/notes.html`.