# Explanation, the Progress of Physical Theories and Computer Simulations

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## Abbreviations

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|---|---|
| CM | Classical mechanics |
| CSM | Classical statistical mechanics |
| CS | Complex systems theory |
| ED | Classical electrodynamics |
| GRT | General relativity theory |
| QED | Quantum electrodynamics |
| QFT | Quantum field theory |
| LFT | Lattice field theory |
| QG | Quantum gravity (in spe) |
| QM | Quantum mechanics (in the text used sometimes as paradigm for quantum theories in general) |
| SM | Standard model: SME (of elementary particles), SMC (of cosmology) |
| SRT | Special relativity theory |
| SST | Solid state theory |
| Th | Thermodynamics |

The ideas developed here have been to no small extent influenced by a long interaction with Heinz-Dieter Zeh and the other members of a FEST[1] project, Domenico Giulini, Erich Joos, Claus Kiefer and Joachim Kupsch. This project led among others

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[2] Joos et al. [32].

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to the book "Decoherence and the appearance of a classical world in quantum theory" (1st edition 1996 and 2nd edition 2003, Springer, Heidelberg, New York[2]) and to a Workshop we have organised at ZiF ("Decoherence, Theoretical, Experimental and Conceptual Problems"[3]) and I am happy to mention here the high intellectual and human capital I drew from the interaction in this group. A brief account of these considerations also entered a talk at the Conference "Mechanistic Explanation, Computability and Complex Systems" of the *International Academy for the Philosophy of the Sciences*, Dortmund, 2016 and extend ideas I have published previously.[4] This essay is dedicated to my daughters.

I want to thank Claus Kiefer for a careful reading of the manuscript and for his important comments and good suggestions. I also want to thank him generally for his engagement and work in bringing forth and preparing this volume. Our group mentioned above went apart many years ago but I still have a good and thankful memory of our discussions. I am indebted to Lukas Barth, a very talented young physicist with both solid mathematical and philosophical interest, for reading the manuscript and for his useful comments. I am indebted to Erhard Seiler for his invaluable help in achieving consistence and improving precision and understandability of this essay and for the time he invested in that. I take this opportunity also to thank my friend and partner in physical projects Erhard for the many discussions and the collaboration we had over many years and his occasionally successful efforts to make me appreciate the depths and abysses of mathematical physics. And finally I want to thank my colleague and long time friend Michael Schmidt in Heidelberg for many discussions and common projects, for his deep physical understanding, and not the least for his personal support since our first meeting 1969.

Both Heinz-Dieter Zeh and Joachim Kupsch passed away in the recent years which was a sad event for many of us.

## 1 Introduction

I propose a discussion concerning the features of explanation in modern physics and also the role of computers therein. My approach is pragmatic and I apologize for unconventional use of philosophical concepts. This approach appears supported by the discussion provided by well known physicists in articles or books—see also the excellent overview by *Erhard Scheibe*.[5] I think this perspective is important for a genuine interaction between physics and philosophy of physics.

Nature is the object of physics and physics the object of philosophy of physics. Therefore it is not only understandable but in fact compulsory that the evolution of physical knowledge should keep opening new horizons to the philosophical understanding, in the same way the former is driven by the study of nature itself. This

[3] Blanchard et al. (Eds.) [9].

[4] I.-O. *Stamatescu* in Ferrari and Stamatescu (Eds.) [22] and in Seiler and Stamatescu (Eds.) [48].

[5] Scheibe [44].

happened in the seventeenth century with the Copernican–Galilean revolution, in the nineteenth century with the establishing of classical physics, in the twentieth century with the advent of quantum physics—with corresponding changes in our world view and new perspectives in the philosophy, cf. e.g. the discussion on causality in *E. Cassirer* "Zur modernen Physik".[6] But this also suggests that physics at any stage cannot be fully analysable according to strict philosophical schemes since it must bear the seed of change implanted in it by nature. With Einstein: "The scientist … cannot afford to carry his striving for epistemological systematics [too] far. He accepts gratefully the epistemological conceptual analysis; but the external conditions, which are set for him by the facts of experience, do not permit him to let himself be too much restricted in the construction of his conceptual world by the adherence to an epistemological system."[7]

The philosophy of explanation is a far developed field with many streams—between a "realistic" line supported, say, by Salmon[8] and an "epistemic" (anti-realistic) line represented by Hempel,[9] branching in a wide landscape, and also including computational,[10] cognitive,[11] communicative, and other models. The Theory of Explanation is a very interesting topic in the frame of the philosophy of science. It aims at analysing the structure itself of what we want to call explanation and the consistency, the a priori basis and the achievements of the various models. It typically tries to reach a general understanding of explanation over the borders of particular sciences and to abstract in this way its essential character. This will not be, however, our approach here as hinted at in the above remarks. First, we shall concentrate our discussion on physics (and I hope—but do not claim—that we can obtain here paradigmatic insights). Secondly, we shall not start from one of the many philosophical explanation models and try to apply it to physical theories. I want instead to start from physical theories, their features and their progress and try to see in what sense and how can we then speak of explanation. This should also give us the means to follow the development of physics, which I assert to be an essential aspect in a discussion of explanation. This is a bottom-up approach as compared to the top-down one of the philosophical discussion. I do not intend to define an "interface" between these approaches, but there may be some hints to take from each other. So, for instance, the coherence question from the philosophical discussion which is not immediate in the bottom-up proceeding, or the wholeness character of explanation implied by the closed systems of concepts of the physical theories which seems not a major point of view in the top-down approach.

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6 Cassirer [15].

7 A. Einstein, "Reply to criticisms", in Cushing [18], p. 357. This is not "against philosophy", this just means that physics needs its free space to do its job.

8 Salmon [43].

9 Hempel [28].

10 See, e.g. Thagard [50].

11 See, e.g. Churchland [16].

My assertion is that the physical theories provide explanations for the physical world and not mere ad-hoc instruments for classifying the observations. In the following I shall try to make this statement concrete.

I shall proceed from the poignant discussion given by Duhem.[12] After renouncing (with him) metaphysical models I shall take as basis for my approach his identified aim of physical theories as promoting "natural classifications" and recognise the latter as "explanations".[13] This of course is not Duhem's concept of explanation which he associates with providing a metaphysical model which he wants to exorcize from physics. The basis of my discussion, sketched here and made explicit in the next sections is summarized in the following two statements.

*I want to consider explanation as that which is produced in (provided by) physical theories and try to discuss the features of the former in terms of the properties of the latter.*[14] Notice that I shall not speak of the particular explanation a certain law provides for a particular phenomenon, unless this represents a valid specialization of the theory or of a closed approximation to it. The interesting object to consider in connection to explanation is the theory as a "consistent system of concepts" (Duhem thesis).

*I contend that realistic points of view understood as the claim that physical concepts—or physical symbols,* Sect. 2.1*—have a referent in the real world are perfectly defensible.* Although in the evolution of the physical knowledge both the symbols and the "objects" they are supposed to refer to change, a steady referential correlation exists, is well defined and follows the evolution of the theories. Correspondingly, explanation is to be seen as a process which can itself be understood from the evolution of the theories.

Thereby I shall make a number of qualified omissions. I shall not present a critical discussion of the relation between experimental results and observations on the one hand, and what we shall call "empirical facts" on the other hand—neither at the level of controlling the former (which we assume fulfilled by standard procedures[15]) nor at the more subtle one of the interpretation of our perceptions.[16] We shall not discuss further procedures in translating empirical facts in mathematical objects, such as idealization and generalization, besides mentioning their role in explanation. We shall not go into details of the physical theories and their progress beyond the aspects most relevant for the discussion intended here. I shall also not enter the philosophical

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[12] Duhem, "La theorie physique, son objet et sa structure" (1908), english translation [20].

[13] A discussion of the understanding of "natural classification" as assumed in the following will be given in Sect. 2.3. For the moment I shall only refer to Duhem [20], Chapt. 2 with the suggestion that the order provided by an accomplished theory tends to be "the reflex of an ontological order".

[14] There are of course also other notions of explanation as related to the context, to other understanding of causation or to particular phenomena—cf. for instance P. Weingarten, M. Massimi in proceedings of the AIPS Conference 2016, "Mechanistic Explanation" (to appear). For a general discussion see Woodward [55].

[15] This implies of course theory and mathematics and can be very complex—the "cosmic distance ladder", for instance, belongs to the empirical part of cosmology but it implies both observation and theoretical models.

[16] H. von Helmholtz, "Die Tatsachen in der Wahrnehmung" (1878) in [27].

discussion of the many models concerning the foundations of physical knowledge and the character of the research. Instead I shall follow Helmholtz, view realism as a good hypothesis[17] and try to see what conditions does modern physics impose on it. I would consider myself as an adherent of a "critical scientific realism", but instead of trying to find a good name for this I shall just let it hopefully become clear in the following.

The most important omission, however, is that I shall only consider established physical theories, going up to the Standard Model of elementary particles (SME, a QFT) and of cosmology (SMC). The latter are called "models" since they do not provide a (sought for) full unification for the fundamental phenomena, not even for the electro-weak and strong interactions. They are seen therefore as steps in an advancing search for unification which eventually should include all interactions especially also gravity. At present we only have a classical theory for the latter which relates gravity with the structure of space–time (General Relativity, GRT). The cosmological standard model SMC is based on GRT but introduces concepts from the SME without achieving a unification of the two theoretical schemes.

In spite of them being considered as models SME and SMC are to a certain degree established and provide a basis for advancing and testing any further developments (beyond searching for solutions in the framework of the SMs, such as dark matter). Some further developments, however, are either limited to the description of a number of fundamental paradigmatic phenomena such as black holes which, however, could not be bound in an overall, consistent theory of Quantum Gravity (QG). Or they belong to a field of partly competing ideas and models such as string theory, AdS/CFT, asymptotically safe gravity or loop gravity which also do not yet build up a unique, overriding and established theoretical scheme. Therefore I found it difficult to recognise and select an overriding symbolic structure, although there are very many exciting developments which also involve new mathematics. It might be that explanation starts now exploring new directions with a new hypothetical basis of metaphysics and principles, however I could not provide interesting speculations beyond those already populating the field. It is not even clear in some cases that my approach of seeing in theories the achievement of a "natural classification" can be meaningful unless we take a platonic perspective.[18]

I shall also not discuss other *Ansätze* particularly concerning QM for which a deterministic metaphysics is postulated. Among the furthest studied are the de Broglie-Bohm model[19] which uses a non-local process and 't Hooft's classical cellular automaton model.[20] Likewise I shall not discuss unifying *Ansätze* based on an universal quantum theory of matter and mind (*Geist*), such as Görnitz and

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[17] H. von Helmholtz [27]. In modern terms his argument can be described as IBE (inference to the best explanation)….

[18] Tegmark [49] and related papers. This perspective can appear as the logical completion of a certain form of "structural realism" which appeals to mathematical physicists such as Poincaré and Weyl and which cuts short the question why, say, equations and the objects they both define and refer to should have different ontological status.

[19] See Bohm and Hiley [12], also Bell [5].

[20] For a comprehensive account see 't Hooft [51].

Görnitz [25] which display a monist entirety picture of everything in a development connecting to the "Ur-model" of C.F. [52]. All these competing approaches introduce various metaphysics. As interesting as these developments and those mentioned before can be, such discussions need a different frame than the one provided by this essay.

In the first two sections of the first part I shall briefly discuss some relevant features of our theories and their progress, before approaching in Sect. 3 the connection to explanation. In Sects. 2.4–2.6 I shall go into some detail concerning aspects of this connection and how this is reflected in our view of explanation. Section 2.7 is a brief recall of the so called decoherence, both because it enters some of the arguments in the main discussion and because it was the basis of the common work in the project with Heinz-Dieter Zeh mentioned at the beginning. Section 2.8 addresses the role of mathematics in theoretical physics and Sect. 2.9 closes the discussion.

As I try to convey in the first part an important aspect is the mathematical structure of physical theories.[21] This aspect follows from a basic interaction between physics and mathematics. Physics uses mathematical schemes, but many developments in mathematics are prompted by physical questions. One essential feature of the role of mathematics concerns the fundamental quantitative aspect of physics. This introduces computation and computability as indispensable components of this structure and computers as their major basis. This will be the subject of the second part of this essay. We shall see there a sketch of the various uses of computers in physics and of the further developments concerning both use and definition of computing. Finally I shall discuss how the participation of computers in explanation may be viewed.

# 2 Physical Theories and Explanation

## *2.1 Physical Symbols and Physical Theories*

*Symbols and physical knowledge; The character of physical symbols; Theories as closed conceptual systems*

For a discussion of explanation in physics I propose to see symbols as the basic elements in building physical knowledge. I prefer the notion of symbols to that of sign and of concept: the symbol points at some thing (like a sign) but also bears[22] an inner structure (like a concept) allowing it to connect to other symbols. This is rather akin to what Leibniz says about ideas and the capability to build ideas as fundamental

[21] In fact this interaction reaches also the meta-theoretical level when comparing different theories, cf Barth [4].

[22] Or indicates a structure which can be deployed when asked for.

for thinking: … there must be something in me which not only leads to the thing but it also expresses it."[23]

A succinct modern history of symbol is given in the article "Sources for the history of the concept of symbol from Leibniz to Cassirer" by Massimo Ferrari.[24] Particularly intuitive for a physicist is the proposal of Heinrich Hertz" We construct internal appearances or symbols of external objects, and we make them such, that what results by thought-necessity from such symbols will always be a symbol of that what follows by nature-necessity from the symbolised objects …".[25] This frequently is referred to as a constructivist testimony whereby it is overlooked that one speaks here of "symbols of *external objects*" (Hertz) —which the symbols "*express*" (Leibniz). In the following I shall stay at the above pragmatic level and sometimes also use the word physical concept meant however as symbol.

Of course one can ask which are, say, the "things" mentioned above, what is their status, etc. A discussion of this and other aspects of the use of symbols in physics is provided in the mentioned volume *Symbol and physical knowledge*[26] which is dedicated to this approach and collects contributions from philosophers and physicists.

Physical symbols appear and act in the process of evolving physical knowledge, they however "solidify" in the frame of theories, when the process finds its realisations in "closed systems of concepts (or symbols)".[27] It is therefore useful to primarily refer to physical theories. For definiteness we shall mostly stay within the so called "fundamental physics",[28] that is the theories of fundamental phenomena where some of the problems to be discussed appear most clearly.

First let us notice that the physical symbols are bound in a network of connections with two main valencies: On the one hand, they have to support the abstract, *mathematical structure* of a theory as expressed, e.g. in the equations of the latter. Therefore they need to be defined as mathematical quantities. On the other hand, they must support the *interpretation* of that abstract scheme down to phenomena and therefore must act in logical chains of symbols aiming at experiment and observation. We thus must define measurable quantities and measurement or observation rules. A rude illustration is given in Fig. 1.

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23 "… es muss also etwas in mir geben, das nicht nur zu der Sache führt, sondern sie auch ausdrückt." see Leibniz, Quid sit idea", in C.I. Gerhardt (Ed), vol. VII, p. 263 sq. [24].

24 In Ferrari and Stamatescu (Eds.) (2002) [22].

25 "Wir machen uns innere Scheinbilder oder Symbole der äußeren Gegenstände, und zwar machen wir sie von solcher Art, daß die denknotwendigen Folgen der Bilder stets Bilder seien von den naturnotwendigen Folgen der abgebildeten Gegenstände …" [30]. Notice that this parallels Leibniz' conception, which is also worth mentioning: "Dass eine Idee von Dingen in uns ist, heißt deshalb nichts anderes, als dass Gott, Urheber gleichermaßen der Dinge wie des Geistes, diese Fähigkeit des Denkens dem Geist eingeprägt hat, damit ⟨derselbe⟩ aus seinen Tätigkeiten dasjenige ableiten kann, was vollkommen demjenigen entspricht, was aus den Dingen folgt." in C.I. Gerhardt (Ed), vol. VII, p. 263 sq. [24].

26 Articles in Ferrari and Stamatescu (Eds.) [22].

27 W. Heisenberg, in Scheibe and Süssman (1973), p. 140 [45].

28 For an actual assessment see Seiler and Stamatescu (Eds.) (2007) [22].

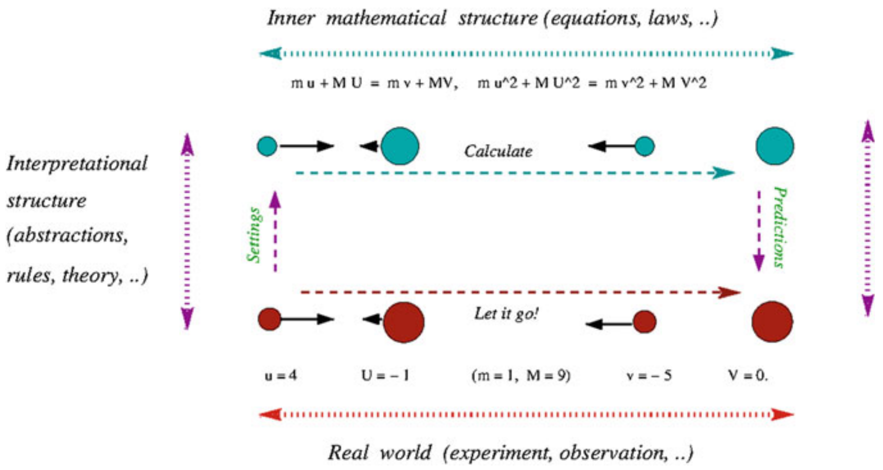


**Fig. 1** Abstract collision with a slow lorry in an extended Hertz scheme. © by the author

Now, the evolution of physical knowledge as we can follow it, say, since Galilei and Newton (and if we discard some few dead ends like *caloric*, *phlogiston* or *ether*) appears to proceed by producing systems of symbols which are closed within a mathematical scheme and over a class of reproducible phenomena well defined by general criteria (e.g., scale, type of interactions, complexity). This evolution is not cumulative but progressive in that it produces hierarchies of theories with increasing capacity of reducing the multiplicity of the phenomena to few rules (laws). In such hierarchies the theories remain related in the sense that the "lower" theory can be approached in the frame of the "higher" one.

We have as *fundamental theories*: *Classical Mechanics* (CM), *Thermodynamics* (Th*), Special Relativity* (SRT) and *General Relativity* (GRT), C*lassical Electrodynamics* (ED), *Quantum Mechanics* (QM), *Quantum Electrodynamics* (QED) and the *Standard Models of Elementary Particles* (SME) and *of Cosmology* (SMC)- which involve particular cases of *Quantum Field Theories* (QFT).[29] Directed at the description of complexity is S*tatistical Mechanics* (CSM) and more generally the *Theory of Complex Systems* (CST). *Solid State Theory* (SST) uses QM, ED and CSM to build up a theoretical scheme defined by its domain of application. In the following I shall refer to QM as a paradigm of quantum theories, unless I shall explicitly consider one or other particular quantum theory.[30]

The line ED—QM—QED is a particular example of the evolution of theories and their symbolic structures. In all three we have, e.g., a symbol for the *electron* as a

[29] The SM are in fact a collection of partial QFTs without complete unification, GRT and partial models.

[30] A succinct presentation of the features and the general implications of quantum theory including most of the themes discussed here is Kiefer [34], see also Kiefer [33] for a brief introduction and discussion of the main quantum effects.

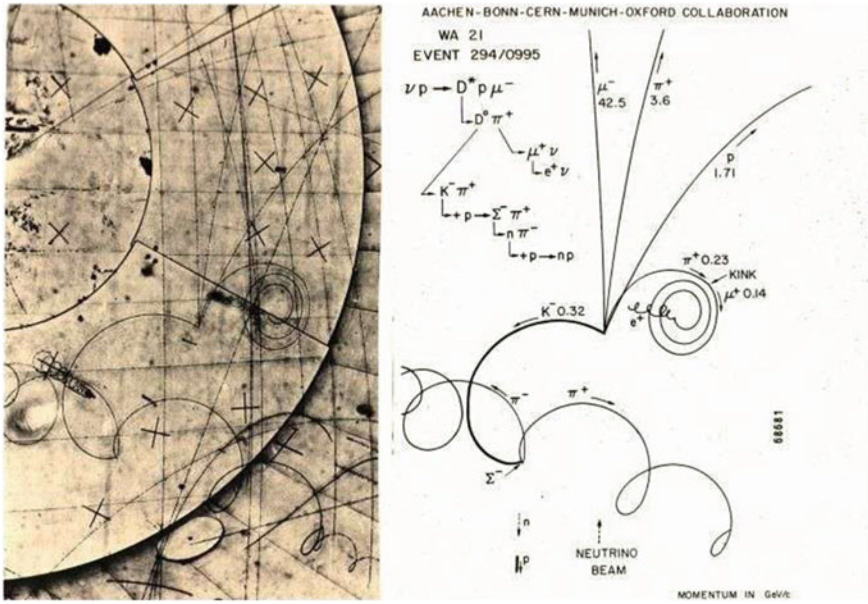


**Fig. 2** Bubble chamber BEBC event, Dec. 1978, D-meson, © 1978–2017 CERN

fundamental object of the theory. It is typically indexed by $e$, but it clearly does not have identical properties in the different theories. We find:

$e^{\mathrm{ED}}$: classical particle, identifiable, conserved, obeying SRT.
$e^{\mathrm{QM}}$: quantum particle, not identifiable, conserved, obeying CM (Galilean symmetry).
$e^{\mathrm{QED}}$: quantum particle of a quantum field obeying SRT, not identifiable, not conserved.[31]

In an absolute sense these symbols have no unique referent. However, from a pragmatic point of view in an empirical and a theoretical sense they directly address reality: they are well defined in the frame of each theory and point each time onto a reproducible empirical fact of a class of phenomena well defined by general criteria. They are compatible by connecting to each other, especially when a "higher" theory overrides a "lower" one, incorporating its empirical domain giving its limitations and developing its symbolic scheme.

This is nicely illustrated in Fig. 2 which represents a celebrated bubble chamber event (evidence of *charm*) at CERN. We see on the same picture production of particles (a QFT effect) which then produce traces in the medium (where also *decoherence*

[31] In fact $e^{\mathrm{QED}}$ is not really a fundamental object in the theory. The fundamental objects in QFT are the quantum fields, in which the fundamental relations of the theory (local interactions) are expressed. Particles are special manifestations of the fields. We also have unstable particles and resonances (e.g., Higgs boson!) and we observe a continuous transition between what we understand by particle and by just signal (enhancement) in a collision cross section. See also Falkenburg [21].

*plays a role,* a QM effect, see Sect. 2.7) and move according to *classical* ED in the superimposed magnetic field.

Based on these observations, the proposal is:

*When conceptual systems close in coherent, successful theories over a class of phenomena (Heisenberg) they define a symbolic structure and symbols having a conditional claim for reality (referential properties), necessity, truth-carrying properties, relative to a both theoretically and empirically well circumscribed and reproducible class of phenomena (typically defined by the energy scale).* The theory as a whole inherits the above properties. We shall speak therefore of a conditional character of the theories relative to a given step in the development of the physical knowledge.

Notice that the symbols show certain continuity properties in the theory developments and generalisation capabilities: e.g., in proceeding from QM to QED we use the symbols $e^{\mathrm{ED}}$ and $e^{\mathrm{QM}}$ as basis for developing the new symbol $e^{\mathrm{QED}}$. We even use the symbols of QM particles as generalized to unstable particles observed as "resonances" in collision experiments. These symbols also seem to build up a ladder in their capabilities to describe the phenomena, therefore we may ask whether they might represent milestones on a track, let us call it $e$ leading our search. Whether this track converges and onto what is a good question: it may completely change its character or be replaced by another concept. We don't know whether a *Final Theory* is possible and if it will entail an $e^{\mathrm{FT}}$ symbol. But at least for a while this track appears to be a good conception and represent an "element of reality" with its stages having well defined referential relations.

The referential relations, however, are more complex than apparently suggested, for instance in connection with the ED-QM-QED line above. The electron, say of QED, $e^{\mathrm{QED}}$ is a very complicated object which reveals its properties in the relations to the other symbols of the theory. These include its participation in the mathematical-conceptual structure of the theory as well as in relating to empirical observations. It is a basic effort to define its predicted properties as well as to envisage and perform the corresponding experiments. Such is, for instance the spin-magnetic moment of the electron which is by a so called gyromagnetic *g-factor* larger than its classical value. The relativistic, quantum mechanical Dirac equation gives $g = 2$ which already fullfils certain empirical bounds and the overriding quantum-field theory QED gives a correction $g\text{-}2 = 0.0023193048(8)$ agreeing to 13 digits with the refined experimental value 0.00231930430256(13)! The referential relation is dynamical, paralleling the evolution of the theories and of the empirical performance. This also emphasises the role of calculations.

Each of the mentioned fundamental theories is closed in its mathematical and interpretational scheme and also concerning its empirical reference domain.[32] It

[32] The notion "closed" as used here is rather sloppy and does not imply that the dynamics may not lead to "unphysical" situations, such as singularities and divergences. Sometimes these can be tamed by supplementary procedures, as in QFT, but they also can be of a more fundamental nature, as in CM, ED or GRT and signal the need for an overriding theory.

provides a good description of the phenomena in some restricted validity domain as a controlled approximation of an overriding theory, so for instance *Newtonian mechanics* (CM) as approximation to *Special Relativity* (SRT) or approximation scheme for the *General Relativity* (GRT)—the so called post-Newtonian approach. Moreover it contributes to the lines of theories' development by providing symbols and symbolic schemes which can be further evolved (Lagrangean, action, equations of motion,..). It is significant that all the theories mentioned above belong to the normal curriculum of the physics study, which stresses the special continuity of physical knowledge.

To summarise: Introducing symbols as basic elements for our discussion helps us in describing physical theories and the way they may be said to address reality. These symbols are bound in a network of relations carrying both the mathematical and the interpretational structure. Following the evolution of our physical understanding we need to qualify the referential features of these symbols and thus also the relation of the theories to physical reality. A brief account of this evolution is sketched in the next section.

## *2.2 On the Progress of Theories*

*Principles, symmetries, scales and thresholds*

Some arguments oppose a view, that physical theories proceed by "accumulation", to one of sudden "jumps". This "myth" grossly simplifies the situation. Physical theories never develop just by accumulation and also never simply make jumps. *Ptolomaeus*' system developed by accumulation, but this was not a theory. The electrodynamics before Maxwell was not a theory either, but a collection of partial findings.[33] Special relativity was the work of a genius, but it was motivated by *Maxwell's Electrodynamics* and came in a context of very many ideas and results (*Lorentz transformations,* etc.). The myth resides on a misunderstanding: on the one hand, accumulation of facts and ideas is a necessary step *before* a theory can emerge. This accumulation is provided in partial findings and laws (Kepler, Coulomb, Faraday,..), in tests using the old theories (such as black-body radiation) or in unexpected empirical facts (radiation, beta-decay). On the other hand, once a theory is established we still have to find and test its consequences for all possible situations—such as describing the movement of a number of bodies in gravitational interaction, or the mass-spectrum of QCD. A theory is typically given by a limited number of relations and we must decode its inner structure to apply it to phenomena. This work is accumulation of information *about and from* the theory, and it will also help us to find its failures[34] and

[33] This accumulation was the ground on which Maxwell's ED could be established, but the latter is not just the sum of these partial laws. Accumulation and jumps are strongly intercorrelated, a modern example is the development of the SME.

[34] Theoretical (e.g., the divergent self energy of electrons) as well as empirical (e.g. the stability of matter) in ED.

proceed to a new level of physical understanding. It prepares the field on which new ideas can be born and based on new empirical findings ingenious work would realise a *jump* to a new theory. We found, for instance, that Newtonian gravitation cannot describe the internal movement of visible matter in galaxies. The main present work in this connection is testing hypotheses for dark (unvisible) matter or for modified gravitation laws which should show whether an extrapolation of old symbols may work or new ideas are called for. The evolution of theories is a process with interacting empirical and theoretical steps. An essential step is *promoting hypotheses*. Besides empirical information and theoretical indications we are helped here also by some general principles.

For Aristotle principles are the foundation of knowledge.[35] Ernst Cassirer speaks of principles as the matrices for building laws of nature.[36] In the present day physics principles are indeed used in establishing laws of nature and constructing theories. However, they may depend on the context in which they are introduced and may sometimes be replaced by a different concept. For instance, the shortest path principle of geometric optics (expressing the minimal action principle of Maupertuis) is not needed in wave optics, where using Huygens principle and the formation of wave fronts leads to the same and many more other results from interference effects in the propagation of the light waves.

Among the principles acting in establishing physical theories a primordial role is played by symmetries. Symmetries are statements about the invariance of physical laws under certain kinds of transformations. The most evident symmetries concern space–time, so for instance the *Galilean symmetry* of CM (translations, rotations and uniform motion) or the *Poincaré symmetry* of the so called *special relativistic* field theories (ED and QFT). Less intuitive are the so called internal symmetries, especially the so called *local gauge symmetries* which can be understood as a certain freedom in locally defining a field while ensuring comparability of fields at different points by transporting information of the local properties from point to point.[37] In establishing the *Standard Model* we found how such symmetries can be combined, and in searching for a so called *Grand Unified Theories* (GUT) how they can be derived from higher symmetries.

One interesting symmetry in the evolution of theories corresponds to *scale transformations*. To introduce these transformations we must first speak of "dimension" (as measured in meters m, seconds s, Joule J or eV). The existence of universal laws and fundamental physical constants which are pure numbers implies that we can translate the various units into each other. This brings in the so called *natural units system* in which there is only one "dimension", say the *length*, and all the others are

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[35] Barnes [3], Aristotle, JB 53::Analytica posteriora I 2 71b.

[36] Cassirer [15], p. 189.

[37] This concept was hypothesized following the empirical observation of conservation laws (e.g. charge conservation) and other correlations between observations. It led to a powerful theoretical *constructive principle*. It is not a genuine symmetry but has rather the status of a *covariance* since physical information is normally carried by gauge invariant quantities.

powers or inverse powers of it. The *energy*, for instance, is an inverse length and typical units like GeV (about the rest energy of a proton $=1.6021773 \times 10^{-10}$ J) and fm ($= 10^{-15}$ m, about the "size" of a proton) are related by 1 GeV $\times$ 1 fm $\simeq$ 5.068. Scale may refer to length or to energy. Scale symmetry (invariance under scale transformations) would appear as scale independence of certain phenomena or theories not involving dimensional parameters (lengths or masses).

We have before differentiated theories by the scale of phenomena to which they apply, for instance CM—QM—QFT, or CM—SRT by increasing the *energy scale*. This however, was not precise enough.

Firstly, the domain of phenomena addressed by the higher theory includes that of the lower one. The latter domain can be efficiently approached in a sufficiently good approximation by the lower theory while the higher theory is valid "everywhere" in the enlarged domain.

Secondly, scale transformations are continuous transformations, while the chain of theories is discrete. In fact increasing the *energy scale* we encounter thresholds and the need to introduce new theoretical elements in order to obtain a closed system of concepts. With increasing velocities the *Galilean relativity* of CM became increasingly inadequate but the new theory (SRT) required a new, consistent mathematical scheme introducing a new symmetry (*Lorentz group*). The step from QM to QFT was called for empirically by the (expected and observed) opening of thresholds for particles creation at high energy and theoretically by the necessity of incorporating SRT in the theoretical schemes. But in order to account for this a new theoretical scheme was necessary: not only a new symmetry (SRT) but also a redefinition of the fundamental physical quantities (*quantum fields*) and of the complete mathematical, conceptual and interpretation scheme.[38]

It may be useful for the discussion of continuity to briefly follow the CM-QM-QFT chain. We can indeed reproduce CM effects in a genuine QM analysis (*decoherence*) but not the logical structure of CM. Conversely, the QM scheme is not *deducible* in the frame of CM. Even clearer is the case in the QM-QFT connection, where the change in the fundamental symmetry (from Galilean to SRT) forces a redefinition of the fundamental quantities for which the fundamental equations hold (from *particles* to *fields*).[39]

In a certain sense when a "higher" theory takes over the domain of a "lower" one one can say the lower theory was wrong and if we were clever enough we should from the beginning go for the higher one. But this is not so easy. Take CM-SRT: it would have been a undefined procedure to look beyond CM without any theoretical or empirical hints, and it would also be cumbersome to approach phenomena at low

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[38] A relativistic QM cannot be established as a consistent theory see e.g. Wachter [53]. This makes clear that one cannot simply add a new hypothesis to an old theory but one must build up a new, closed theoretical scheme "incorporating" the former. In the case at hand it means going from particles to fields as fundamental with particles as a manifestation of these.

[39] We can, however, on the basis of a given theoretical scheme valid at a high energy scale derive *effective theories* at lower scales by the "renormalization group" procedure which allows to redefine the theory for adequate applications there.

velocity, easily described by CM due to the Galilean symmetry, with the full SRT arsenal. CM is a necessary step before and a useful one after SRT. Even worse is the case for the CM-QM pair. Here we need to determine a whole process (decoherence) besides taking limits in order to obtain a description for phenomena like scattering of particles or moving in an external field.

But there is more to it. The logical structure of each theory in a pair is evolved on the basis of a class of phenomena it is confronted with. The success of these theories means that *nature does behave that way there*. In my brand of a "critical realistic" view the symbols of these theories find their referents there. Therefore in the progress from lower to higher theories we just follow the sometimes complicated build up of nature itself. It is nature which suggests to us closed theoretical schemes since it apparently follows a hierarchical structure—which should then be mirrored in the progress of theories. And developing the lower theory is indispensable also because this offers symbols to be further developed.

Before proceeding, however, to relate theories and explanation we should say a word about identifying objects. Again, this discussion does not belong to the philosophy of science,[40] but to physics. Most symbols in a theory can be seen as "objects" and we may ask how are these objects identified (which implies both finding and constructing them, see below). Many of them are intuitively found as chunks of matter (e.g., the particles mentioned in Sect. 2.1) or of energy (e.g., the photons) but they may also be subject to metamorphoses, so is, for instance the "force" of classical physics and of QM replaced by the exchange of certain particles in QFT. As already suggested by these comments—and by the discussion of Sect. 2.1—identifying these objects is itself a process between experimental observations and theoretical hypotheses ending up in a consistent symbolic network which is the theory with its mathematical, interpretational and empirical structure. Here a role is also played by metaphysical conjectures and the "continuation" of objects from other (typically preceding) theories, metaphorical suggestions, models, etc.—but the last word is said when the complete scheme of the theory closes. The processes of object identification are included in the progress of theories.[41]

## 2.3 How Do We Understand Physical Theories and the Question of Explanation

*Features, status and the development of a theory; What does a theory achieve; Explanation and natural classification; Explanation and physical theories*

With the previous discussion in mind we can now proceed to make the connection to explanation and substantiate the assertion in the introduction. As already suggested there we consider explanation as provided by mature theories. A theory is a self

[40] For a brief overview see Rettler and Bailey [42].

[41] For a transcendental perspective see Bitbol et al. [8].

consistent, tight conceptual scheme with a mathematical inner structure and laws for relating its symbols to observation. These are fundamental aspects, since only then can we comply with the requirement, already voiced by Aristotle, that knowing means to know the grounds by which some thing is and also know that it cannot be otherwise.[42] A theory must claim necessity and universality with respect to a well defined class of reproducible phenomena, since only then can we learn, from agreement and from disagreement, and evolve our knowledge.

A theory may be built upon a number of (partly already established) partial rules and laws which it binds in a self consistent overriding scheme. The theory is more than the sum of these partial laws. Consider as example *Electrodynamics* (ED) where this can be observed in detail: it is preceded by the laws of electrostatics (*Coulomb*), currents (*Ampère*), induction (*Faraday*), ... but it is the genius of Maxwell to put forward the universal scheme of ED. This is now a coherent, tight scheme. It is significant, for instance, that this scheme introduced, for purely mathematical-theoretical reasons, a new law which could not be guessed from the partial ones (the *displacement current*). As a result a resetting of the space–time symmetries was promoted which finally led to Einstein's SRT. Another new result was the identification of light and electromagnetic waves.

The logic of the theory development is to follow the "how" (directly related to observation and based on induction) to a "why" (receded from observation and based on hypotheses). Thereby the multitude of observations typically gathered in empirical laws is *reduced* to few fundamental laws: From Kepler's *kinematic* laws describing the movements of the planets to Newton's gravitation theory which introduces the *dynamical* universal attraction law of gravity and from which Kepler's *kinematic* laws can be *derived*; from the laws of atomic spectra (Lyman, Balmer, Paschen) and of the black body radiation (Rayleigh- Jeans, Wien, Planck) to QM.

As argued in the previous sections we must and can refer to the theories closing as conceptual systems at each step with reference to a class of phenomena which give them a conditional (relative) character as discussed in Sect. 2.1.

With this in mind let us ask: What does a theory achieve? Duhem's claim, for instance, is that a physical theory does not provide explanation in the sense of revealing a metaphysical structure, however it also is not just simple classification. It provides instead.

*A "natural classification" of laws and objects, and the better the theory becomes in describing and predicting phenomena, "the more we apprehend that [its] logical order ... is the reflex of an ontological order".*[43]

If we renounce therefore of searching for metaphysical revelation it seems then natural to relate explanation to physical theories and see the task of explanation as

[42] "[wir meinen] etwas zu wissen, wenn wir glauben, sowohl die Ursache zu kennen, aufgrund derer ein Ding ist (und zu wissen, dass diese seine Ursache ist), als auch, dass es nicht anders sein kann" Barnes [3], Aristotle, JB 52: Analytica posteriora I 2 71b.

[43] Cf. Duhem [20], Ch. II, & 4. This and other statements in Ch. II and at other places suggest that the "instrumentalism" positioning of Duhem may need a more refined discussion, as also hinted at in Ariew [2], see also the article of Karl-Norbert Ihmig in Ferrari and Stamatescu (Eds.) [22].

putting into evidence *"natural classifications"* aiming at uncovering the *mechanisms of nature.*[44] The suggestion is therefore.

*to consider explanation to be provided by physical theories and just as these to be committed to an evolutionary process and have at each stage a relative (or conditional) status.*

Explanation in this view is therefore a process: we can "explain the world" at a certain level and can push our knowledge further with the theoretical progress, *resetting* the old explanation in the new frame.[45] And as with the evolution of theories, the older explanation is not lost: it is retrieved, e.g. as approximation and it has helped building the new explanation. Notice that the mentioned relativism is fundamental and not a question of perspective, since it follows from the direct relation to theories. Of course for one and the same theory there may be different assumptions about some kind of metaphysics or "interpretations" of its basis (QM is a good example: collapse, relative states, etc.) which will enter as alternative metaphysics. This is a relativism superimposed onto the basic processual character.

This basic relative or conditional character will also apply to our understanding of "natural classification" itself and also to other concepts such as "natural kinds".[46] In the pragmatic, realistic approach followed here we can think of natural kinds as the basic components of the theory together with their empirical referents. Is $e$ of Sect. 2.1 a candidate for a"natural kind"? We can only speculate whether $e$ is a relevant object in some final theory, if at all reachable. In the perspective of a process character for explanation we may rather consider the family $\{e^{\mathrm{ED}}, e^{\mathrm{QM}}, e^{\mathrm{QED}}..\}$ as a natural kind, searching for (and finding) its actual referent in each actually given theoretical and empirical environment.

## 2.4 Some Aspects of Explanation in Various Theoretical Schemes

*Metaphysics; Principles; Theory and model; Fundamental and effective theories; Special theories*

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[44] Referred to by I. Kant in *The critique of practical reason, Ch.III*, also as "physico-mechanical connections in nature" in *The critique of pure reason, Appendix.*

[45] We can, for instance, derive *classical behaviour* as a certain QM effect *(Decoherence)*, see Joos et al. [32] and Sect. 2.7.

[46] This is of course an important discussion which, however, is beyond the aim of this essay. In ED, for instance, we should consider also the electromagnetic fields as "natural kinds" and possibly also the potentials because of their role, say, in quantisation. This would imply, however, redefining identity, classes, etc. taking into account gauge transformations and then adapt our discussion on their relative character considering the progress of theories. For a succinct overview of the philosophy of science discussion hereto see Bird and Tobin [7]. Here however we shall only retain the observation that natural kinds just as natural classification have the same conditional status as the theories and their symbols, see Sect. 2.1, and are also bound in the process of evolving the physical knowledge and should be empirically and theoretically well defined at each level.

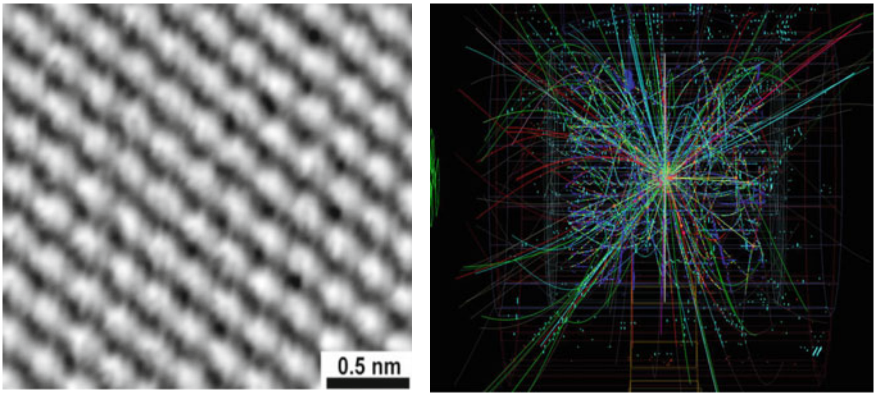


**Fig. 3** **a** *Left*: scanning tunnel microscope picture of a graphite surface showing an ordered lattice of atoms (from commons.wikimedia.org, gemeinfrei). **b** *Right*: high energy LHC event in the ALICE detector, particle shower from a Proton-Pb collision (© 2012 CERN, ALICE)

Relating explanation to physical theories allows us to derive features of the former from those of the latter. One interesting question is, whether metaphysics completely disappears from explanation. If we understand metaphysics hypothetically this is not the case. Instead we find metaphysical settings as basic *assumptions* which can be very efficient in developing theories. An example is the atom hypothesis, which proved very fruitful in leading the development of physics—and one can even reply today to Mach's scepticism ("did you ever see one?") with pictures from field microscope—see Fig. 3 left. A more refined example is that of elementary particles[47]—see Fig. 3, right. Metaphysical settings can therefore enter explanation if we remember the relative and process character of the latter and take into account a hypothesis-character for the former.

A similar situation pertains to principles. Both they and metaphysical settings lead the progress of physical theories and are therefore in some sense "meta-theoretical". As already remarked, however, like metaphysical settings principles may also be related to a certain stage in the evolution of physical knowledge. This will also affect their role in explanation (see also Sect. 2.9).

Other interesting questions concern partial theories, models and effective theories as compared to what we called "fundamental" theories. Effective theories are full grown theories with only the amendment that they comprise a number of parameters and rules which are expected to be fixed at a higher level. As an example, the *standard model* SME is considered an effective theory to be derived from an envisaged more powerful theory with a more comprehensive symmetry at a higher energy scale. The overriding theory should both fix masses and other parameters of SME and provide a higher order of unification (GUT—*Grand Unified Theories*). Correspondingly, the explanation provided by the effective theory is relative in the sense discussed before,

[47] "Particle" is a powerful concept in promoting hypotheses, so for instance it dominates the search for "dark matter". See also Falkenburg [21].

but it additionally acknowledges incompleteness since it refers to another (higher) theory to fill the explanation gaps.

A certain subclass of phenomena can be successfully treated by setting up a theoretical scheme based on the particularities of that subclass of phenomena. Such is, for instance, the BCS-theory of *superconductivity*, which uses ED and QM in a *solid state theory* (SST) frame applied to the special case of the electron flow in some solids at very low temperatures. It identifies special effects due to the coupling between the movement of the electrons and the oscillations of the lattice of ions, introducing new symbols—the so called *Cooper pairs*. It thus provides an explanation in the framing of SST but spelled out for this concrete case. Notice that SST itself borrows basic concepts and laws from QM, ED and *statistical mechanics* (CSM) while also introducing new symbols and rules. The explanatory capacity of the SST implies therefore reference to other theories.

A different situation pertains to models. Many models typically do not represent self consistent theoretical schemes, neither mathematical nor interpretational. Their essential role is to suggest connections among symbols and test hypotheses in a simplified context. Their contribution to explanation is correspondingly sketchy and needs justification through the theories to which they lead or in the frame of which they are developed. The *Bohr atom model* is an example. It is theoretically inconsistent since it is set up in the frame of *classical electrodynamics* while introducing hypotheses incompatible with the classical movement of charges in an electric field—*stable orbits*. However, by suggesting (and testing) these hypotheses it directed the search leading to *quantum mechanics*.

The Landau model for phase transitions in *statistical mechanics* is another kind of example. It is derived from the fundamental mathematical object of CSM (the *partition function)* under some general conditions. It has universality character and can be applied to various concrete statistical mechanics models. It provides therefore elements for explanation of the phenomena due to complexity, independently of the particular interactions involved.

We also find models representing a self consistent approximation of a theory or a reduced account of a substructure thereof with the corresponding subclass of phenomena and aimed at emphasising the role and effect of some relevant connections in the theory, so for instance the non-linear $\sigma$-models or the chiral perturbation theory. Such models can be sometimes transported to other theoretical schemes.

Models have a very important role in the evolution of the theories, sometimes just because their explanatory program is less strong and is flexible enough to take into account analogies and metaphors which are important in building up hypotheses, or because they help selecting dominant theoretical concepts and rules.

## 2.5 Understanding and Explanation

*Explanation and understanding; Intuition; Right concepts*

In my pragmatic view a theory provides *explanation* for the phenomena in its field, and *explanation* as such is well defined. A different question pertains, however, *understanding*. In every day language we say, we explain some physical relations to somebody, but what we mean is making him *understand* them. Let us consider Maxwell's ED. Already the concept of field is not easy to understand. Faraday's concept of field is a very fruitful abstract symbol, his image of lines of force filling the space is intuitive but incorrect: there are two vectors in ED associated with each point in space, varying in a correlated way in time. There is only one vector in Newton's gravity. Intuition and imagination may help a bit but in the end we may need to accept a certain symbol with its embedding into the theoretical structure as fundamental and use imagination only as a vague suggestion to circumscribe it.[48]

*Understanding* and *explaining* are not identical, the former is more complex and less well defined. On the one hand it depends on explanation. So no understanding can come from *Ptolomaeus*' system and not even from *Kepler's* laws since they do not themselves ground theories and thus do not provide explanation. *Newton's* gravitational law (*universal attraction force*), however, does and can therefore bring understanding. On the other hand understanding may precede and generally will interact with explanation. So the concept (or symbol) of *stationarity* introduced in Bohr's model and illustrated by radiation free orbits will become a basic concept in QM. Understanding uses softer concepts than explanation while relying on the latter to give them solidity if required. These concepts are often generated in models preceding a theory (such as Bohr's model) and finalised in the theory or constructed in the frame of a theory (such as the *Cooper pairs* in the BCS-theory of superconductivity). Finally understanding may be context and perspective dependent and therefore not unique.

Being able to describe the simple effects in the theory may be a first step in providing understanding—so, for instance, the two-slit experiment in QM. However, one cannot go far enough this way: most interesting QM effects (*entanglement, decoherence*, etc.) cannot be reduced to intuitive notions and images. Instead, according to *Heisenberg*:

> We have understood a group of phenomena when we have found the right concepts for describing these phenomena.[49]

Finding the *right concepts* is a very important issue, *not only in understanding but in fact already in developing theories and in spelling out explanation*. For that we may need to accept abstract symbols as *"right concepts"*, appearing as nodes in the mathematical and interpretation scheme of the theory. Electromagnetic fields and potentials in ED may be such right concepts. They are not very intuitive (*anschaulich*) but show universality, capability for further developments and underlie a big class of

[48] In a brief section Feynman [23], II, 20–9 discusses the deficiency of the imagination in science while finding intellectual beauty in the wave equation due to the regularities and further developments it suggests. If we take this over to understanding it says that it is not the direct imagination which counts but the multitude of relations implied by a symbol.

[49] W. Heisenberg, "The concept of understanding in theoretical physics", in Blum [10] CIII, p. 335. Notice that "right concepts" and "natural kinds" need not be related.

effects in the theory. These qualities make them also important in the development of theories. The latter selects the adequate symbols for the higher theory, e.g. in going to QED the potentials, which in ED are helpful but not essential, prove to be *the* fundamental symbols for quantisation (local interaction).

Entanglement, superposition, operators, states, measurement are such *right concepts* in QM, some fully non-classical, other distinguished by new properties. There are in fact many further proposals hereto, sometimes as alternatives: the wave function collapse of the Copenhagen interpretation, Everett's relative states, Griffiths' consistent histories, ETH events, decoherence, etc. in various combinations.

Notice that QM comes together with a fundamental break not only in the interpretation scheme but also in its mathematics. Classical physics relies on real numbers, complex numbers may simplify calculations (ED) but are not essential. On the contrary, the mathematics of QM is fundamentally based on complex numbers, starting with the Hilbert space as space of states. This is, e.g. evident in the proof of the *Bell theorem*[50] which also summarises the "picture" of QM showing that the statistics of the latter cannot result from local, hidden variables, which would lead to classical statistics. The difference is made clear by considering a certain correlated experiment and is enforced by the complex number character of the QM quantities.[51] Therefore it may be a bold suggestion to add as a further "right concept" for understanding quantum physics that of complex numbers (complex Hilbert space).

## 2.6 Explanation and the Structure of Theories

*Observation and experiment; Hypotheses; Mathematical scheme*

The building elements of the physical theories are also mirrored in explanation. So we find again in explanation a discussion of the experimental protocols and observational procedures providing the empirical basis of the theory, e.g. the observation of particles in QFT as *tracks in the detectors*, or the *cosmic distance ladder* in cosmology (which both involve theoretical knowledge at various levels). They define the way the symbols of the theory are related to phenomena and thus what explanation pertains to. This also involves the handling of data, interpolation, generalization, etc.

The next step in setting up a theory is the construction of a system of hypotheses concerning the physical quantities and their relations, which define the symbolic structure of the theory. We stressed that due primarily to the mathematical basis of the theory the symbolic structure is a tight scheme and the test of a hypothesis typically involves a bundle of other hypotheses. For explanation this means that we cannot arbitrarily delete or modify an isolated element in the theory and also that we

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50 Bell [5].

51 See I.-O. Stamatescu, Appendix 4, in Joos et al. [32].

must always mention (or at least keep in mind) the complex of symbols and rules accompanying any particular explanation.[52]

Finally, since mathematics plays a key role in physical theories it will also constrain the explanation at various stages: In deriving post- and prediction for phenomena (*celestial mechanics, super-conductivity*); in the search for adequate concepts in the mathematical-theoretical structure of theories (*gravitational waves, quark-gluon plasma)*; by proposing or deriving models *(quark model, Cooper pairs);* in the development of the theories (*symmetries*, *renormalization).* And since physics is a quantitative science this also involves calculations and thus explanation also depends on calculability.

An intriguing aspect relates to the observation made at the end of the previous section. We became used in classical physics to accept increasingly abstract mathematical objects as symbols for the physical objects we want to refer to: vectors for velocity and force, tensors for electromagnetic fields or space–time curvature, etc. We fail to faithfully represent them intuitively (in "Anschauung") but we can give a scheme to "reconstruct" them from our simple intuitions based on real numbers—they remain somehow "familiar".

Not so in quantum physics. The symbols, for instance those for the "right concepts" are defined on the field of complex numbers. This is reflected in the measurement results which are real numbers but fulfil unusual correlations violating the so called Bell-type inequalities.[53]

All this is well and clearly represented as algebraic relations, diagrams, etc. However, it appears difficult to have some representation of the fundamental quantities and relations of quantum physics the same way we do in classical physics and realise a similar familiarity. This may be a reason why we hesitate to accept the "reality" of QM—besides the lack of well defined "conceptual interpretations". But in the view that theories provide explanations and if we do not consider QM as incomplete we may ask which is the "natural classification" QM refers to. Let us assume for a moment that QM offers us a natural classification, and thus leads us to reality, in the relative meaning advanced in Sect. 2.3 (see also Sect. 2.1). Why is this reality, even accepting its relative status and its abstract theoretical representation, so much less accessible to us intuitively than the classical one? We do not even seem aware of the fullness of quantum effects which direct our daily life (starting with the mere existence of the world—the stability of matter).

A simple answer (which might not be wrong) is that QM itself takes care of that. We live in a world of innumerable, uncontrollable interactions which steadily carry away QM phase information. QM *predicts* in this case that as a result the genuine QM effects are damped by *decoherence*[54] and the world *appears* as classical. In fact decoherence may also control the working of our brains and thus our understanding

[52] Cf. the note on relativistic QM (footnote 38).

[53] A metaphysics based on complex numbers is proposed, for instance, in the "Ur-model" of v. Weizsäcker [52], extrapolated to a universal *Ansatz* for everything in Görnitz and Görnitz [25].

[54] Joos et al. [32]. There exist of course macroscopic quantum effects unaffected by decoherence such as superconductivity, laser, transistors with many practical applications.

itself.[55] We always try to use classical concept in every description. We never had the chance to develop “quantum intuitions” based upon complex numbers even in an evidently fundamentally quantum world.[56] The only thing we can do at present is trying to keep in mind the typical effects and quantum laws as an underground world of beautiful beasts, which we only started to tame—see also the last section of this essay. And with increasing penetration of evident quantum effects (such as quantum information, quantum computing, etc.) in our daily life we may also be able to develop basic quantum insights and intuitions.

## *2.7 A Few Words About Decoherence*

Since we mentioned decoherence in various contexts it may be useful to briefly introduce it here, the more so since there were Heinz-Dieter Zeh and Erich Joos who among the first correctly appreciated its importance, both practically and theoretically.[57] It is in fact a standard QM effect, thoroughly studied with its applications in Joos et al. [32], see also Zurek [33, 34]. It is also briefly reviewed in Wikipedia.

For a simple example consider a system *S* built up from two subsystems, *1* and *2,* which each can be in two states, **1** and **1′**, respectively **2**, **2′** like, say, an electron with spin up or down (in some basis). *Classically S* can have just four states and each of them is evidently just one of the pairs, **1 2, 1′ 2, 1 2′** and **2 2′** and in each of these states the two subsystems obviously have well defined states. Quantum mechanically, however, any complex linear superposition of possible states of a system is also a possible state. This ***superposition principle*** holds for *1* and *2* and also for the composite system *S*, therefore any linear superposition of the four pair states above is a possible state of *S*. But clearly such a *generic* state of *S* cannot be associated with a pairing of one state of *1* and one state of *2* from their superpositions.

Consider, e.g., the state $\mathbf{1\,2'+1'\,2}$ of *S*, it is not possible to write it as $(a\mathbf{1}+a'\mathbf{1'})(b\mathbf{2}+b'\mathbf{2'})$, that is as a product of subsystems’ states from the their superpositions (clearly one needs all coefficients *a, a’, b, b’* to be non-zero, but then the product contains unwanted terms..).

55 The hypothesis that quantum effects are at work in our brains, may be problematic since under the typical working conditions there (temperature, external influences) decoherence may be expected to destroy local quantum coherence. In an evolutionary perspective there seems to be no necessity for a quantum organ, see Hepp and Koch [29].

56 There are macroscopic quantum effects which in a sense can belong to daily experience, such as superconductivity, or which by enhancement produce macroscopic effects, such as nuclear energy. And of course X-rays, LED, MRT, etc. They prove that the world *is* fundamentally quantum at all levels but the genuine quantum character is not direct enough to help us build quantum intuitions, and their interpretation remains abstract—the more so that QM itself does not offer us a clear and consistent interpretation for its most fundamental rules, e.g. measurement (albeit when using classical concepts …).

57 There is very much literature on this subject—see, e.g., the bibliography in our mentioned book on decoherence, [32], Therefore I shall only mention some of the earliest studies hereto which also have a direct connection with our discussion here: Zeh [57], Joos and Zeh [31, 32], Zurek [58].

This is ***entanglement*****:** at variance to the classical case there are states of *S* in which the subsystems do not posses well defined states for themselves.

What we observe (measure) in QM are *expectation values* of certain physical quantities *O*, typically called *observables* and the QM rule is to take their "projections" in the system's states, in the above case:

$$
\begin{aligned}
&\left(\mathbf{1}\,\mathbf{2}' + \mathbf{1}'\,\mathbf{2}|O|\mathbf{1}\,\mathbf{2}' + \mathbf{1}'\,\mathbf{2}\right) \\
&= \left(\mathbf{1}\,\mathbf{2}'|O|\mathbf{1}\,\mathbf{2}'\right) + \left(\mathbf{1}\,\mathbf{2}'|O|\mathbf{1}'\,\mathbf{2}\right) + \left(\mathbf{1}'\,\mathbf{2}|O|\mathbf{1}\,\mathbf{2}'\right) + \left(\mathbf{1}'\,\mathbf{2}|O|\mathbf{1}'\,\mathbf{2}\right)
\end{aligned}
$$

Now assume the subsystem *1* to be at our disposal and the observable to refer only to it. Assume *2* to represent the environment of subsystem *1* and after interacting with it go beyond our reach—like, e.g., innumerable particles scattering on *1* and then escaping in all directions. We may then safely assume that these particles no longer care for what happens in our laboratory, or for each other. Their states, here indicated by **2** and **2'** at different edges of the world are therefore orthogonal:

$$
\left(\mathbf{2}\middle|\mathbf{2}'\right) = \left(\mathbf{2}'|\mathbf{2}\right) = 0 \,\text{while}\, (\mathbf{2}|\mathbf{2}) = \left(\mathbf{2}'\middle|\mathbf{2}'\right) = 1 \text{ (normalisation)}
$$

and since our observable *O* is restricted to the laboratory, the result of our observation will simply be.

$$
\begin{aligned}
&\left(\mathbf{1}\,\mathbf{2}' + \mathbf{1}'\,\mathbf{2}|O|\mathbf{1}\,\mathbf{2}' + \mathbf{1}'\,\mathbf{2}\right) \\
&= (\mathbf{1}|O|\mathbf{1})\left(\mathbf{2}'\middle|\mathbf{2}'\right) + \left(\mathbf{1}|O|\mathbf{1}'\right)\left(\mathbf{2}'|\mathbf{2}\right) + \left(\mathbf{1}'|O|\mathbf{1}\right)\left(\mathbf{2}'|\mathbf{2}\right) + \left(\mathbf{1}'|O|\mathbf{1}'\right)\left(\mathbf{2}'|\mathbf{2}\right) \\
&= (\mathbf{1}|O|\mathbf{1}) + \left(\mathbf{1}'|O|\mathbf{1}'\right)
\end{aligned}
$$

This is ***decoherence*****:** it destroys the effect of entanglement in a local observation. This implies *classical behaviour* since the result of our observation is described by classical statistics over well defined states of subsystem *1*. This is also effective in any process in which entanglement would be relevant.

Decoherence is a widely discussed topic. I took the risk to bore the reader in order to stress that this effect is obtained in a standard QM analysis independently of any "metaphysical interpretation"[58] of QM: Copenhagen collapse, Everett relative states, Consistentthistories, ETH events, etc. It involves but does not "solve" ("explain") any of the basic QM postulates (measurement, probabilities), however it is frequently used to ensure consistency of some hypotheses in one or other interpretation.[59] The essential aspect is, however, that it allows quantitative estimates[60] which is important in applications.

One important application concerns quantum computing. Here entanglement is the key factor and the functioning of a quantum computer relies on ensuring stable

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[58] This is not the interpretational structure mentioned in Sect. 2.1 but the attempt to provide a metaphysics for QM.

[59] See, for instance, Zeh [57] and the discussion in Joos et al. [32].

[60] See e.g. Joos et al. [32].

entanglements for the time needed for a computation. This means, however, one needs to evaluate and limit the decoherence effects by good shielding, very low temperature, etc. The presently achieved coherence time is of the order of seconds for a few q-bits. Generally, any process based on QM coherence must take into account decoherence.

Decoherence enters our discussion of explanation in a number of ways.

- By showing that classical observations can be accounted for in QM, decoherence stresses the universality claim of the latter.
- The involvement of the decoherence arguments in "interpretation" proposals such as Everett's relative states or the coherent trajectories stresses its meta-theoretical role.
- Decoherence provides an explicit connection between CM and QM going beyond formal proofs such as the Ehrenfest theorems. It thus confirms the continuity in the progress of theories and at the same time qualifies it by fixing the theoretical and empirical conditions under which we can observe and how we must understand it.
- Since it is a quantitative effect it can be continuously tuned between quantum and classical observation, for instance by varying the vacuum or the temperature in an experimental set-up to observe QM interference. Thus we can understand both the empirical and the mathematical aspects of this effect and how it describes a continuous "transition" between quantum and classical phenomena.

## *2.8 On the Role of Mathematics in Physical Sciences*

*Foundation; Basic roles; Calculation*

As a final point we should speak of the role of mathematics in physical theories, since this role can be taken one to one in the question of explanation in physics.

1960 Eugene Wigner wrote a beautiful small paper *"The Unreasonable Effectiveness of Mathematics in the Natural Sciences"*[61] Of course stressing the essential role of mathematics in physics is a constant issue in the historical development—…, Roger Bacon, Galileo Galilei, Pierre Duhem, Ernst Cassirer, … such that it is taken as self evident. But the interesting question this paper addresses is: why (and how)? I shall not present this paper here and leave to an interested person the pleasure to read it himself (if he did not already do it). I shall only sketch a few of its main arguments.

It starts from some *basic observations*, such as:

[61] Wigner [54].

– Nature shows regularities and this implies that there are laws of nature and that we can obtain knowledge of them. This is the assumption—postulate (*Peirce*), *lawfulness* of nature-hypothesis (*Helmholtz*), general causality principle (*Cassirer*), …—explicitly or implicitly made by most physicists.[62]
– It is possible to select restricted sets of phenomena for consideration within arbitrarily good approximation (approximate *separability*). Electromagnetic and gravitational effects for instance can be separately studied in corresponding experimental design. The legendary experiment attributed to Galilei needed separating the dominant effect (free fall) from disturbances (air friction). And we can give procedures to control the approximation.
– It is possible to use idealization, generalization and other procedures permitting to translate the experimental findings into physical quantities (symbols) adequate for the mathematical treatment and to compare the predictions of the theory to phenomena.

I just wanted to recall the conditions by which in Wigner's account mathematics enters physical theories. In fact an assumed deep compatibility between our thinking and *"the mechanisms of nature"* hinted at here has led to many discussions[63] including the suggestion that our theories just discover the Platonic algorithms which are at the basis of these mechanisms.

The paper then counts *basic roles and aspects* of mathematics in natural sciences:

– Mathematics is a *language* providing basic concepts in formulating theories (*e.g. state spaces, operators*), providing the rules for connecting these concepts into a theory (*equations, limiting procedures*) and of course for handling the empirical information and translate theoretical pre/post-dictions into measurable effects. Mathematics also provides the tools for connecting and developing theories (*symmetries, scale transformations*) and formulating and testing hypotheses.
– Since mathematical concepts are "transportable" mathematics allows the development of new theories by developing the mathematical-symbolic scheme of older theories (e.g., *in proceeding from CM to QM: Hamiltonian, Lagrangean, symmetries*). This also allows the application of a conceptual scheme to different physical situations (*thermodynamics, complex system theory, phase transitions, universality*).[64]
– Since mathematical structures build up an universe for themselves[65] they can be used for completing theoretical schemes or for envisaging new ones in the absence of direct empirical evidence (*displacement current in Maxwell's eqs. —from*

[62] To what extent does QM comply with this understanding of lawfulness is an outstanding question—between the incompleteness criticism (*Einstein*), the claim of universality of statistical laws (*Schrödinger*), the denial of the need for space–time description (Anschauung; *Heisenberg, Cassirer*), ….

[63] See, e.g., the exciting discussion in Penrose [40].

[64] The mathematical-symbolic schemes of classical physics, for instance, provide keys for developing symbols for the newer theories.

[65] See, e.g., Bourbaki [13].

*symmetry considerations, conservation laws; string theories, super-symmetry—in the search for QG*).

Such observations, however, also make clear that we must be able to use the mathematical schemes. Since physics is a quantitative science this means among others that we must be able to calculate. One speaks in this connections of *analytic* and *numerical* procedures.

A good part of the mathematical work of the previous centuries concerned the development of analytic procedures: special functions *(e.g. the well known Bessel functions)*, algorithms *(for solving equations, stochastic processes)*, ... They have provided important insights in physics (*planet trajectories in classical mechanics, simple atoms in quantum mechanics*). However they come to their limits: -With increasing complexity of the problems *(already the 3 body problem in Newtonian gravity has no general analytic solution; complex atoms in QM; phase transitions in QFT and Complex Systems, ...)*. -With the demand for high precision *(celestial mechanics, satellites, Rosetta mission, LIGO detector for gravitational waves, ...)*. Analytic studies today are especially used in models or approximations.

Numerical procedures also have a long history and in the mid of the twentieth century logarithm and Bessel function tables were still in use. However also computing machines started developing since the nineteenth century. And this development acquired in the last decades an extraordinary momentum concerning the capabilities of the machines, which also triggered an exploding field of applications, not least in science. Computers enter now the scene of natural sciences and this will be the subject of the second part.

## *2.9 Closing the Circle*

Relating explanation to physical theories led us to derive a number of features of the former. We thus had to acknowledge a conditional character for the necessity, truth and reality which we can associate to explanation, relative to a (theoretically and empirically) well defined class of reproducible phenomena. We correspondingly have also seen explanation as an evolutionary process, both in its symbolic content and in its structure concerning the different procedures following from the relation to theory development, such as induction, abduction and deduction. That in connection to explanation mathematics is important, even at the meta-level of comparing theories and illuminating the lines of theory development.[66] And finally that an essential role is played by calculations which opens a window toward the role of computers and the revolution happening here.

We have considered explanation as provided in physical theories. We proceeded from physical theories to characterize it. We can accept that a particular theory provides a partial explanation for the physical world. Is explanation just the sum of

[66] This is of course a relevant issue in the philosophy of physics. For a nice example of using modern mathematical tools at the meta-theoretical level see, e.g., Barth [4].

what is provided in the particular theories or is there something more we can say about it? In fact there is also a reverse flow from explanation to physical theories. Explanation tries to produce a coherent picture and thus supports meta-theoretical perspectives. Such are for instance the unification and reduction as "regulative ideas"[67] in advancing theoretical knowledge, but also constructive principles "found on the way" such as "gauge symmetry"[68] or the cosmological principle. In that sense explanation synthesises the theoretical development and at the meta-theoretical level also reveals the features which may play a role in guiding the progress of the theories.

In a realistic perspective the same way we think *accomplished theories* and the explanations they provide have an ontological connection which ensures them a high level of success, we can think that the explanation accompanying the *progress of theories* also has access to an ontological order, because it acknowledges well defined steps and follows a well defined development "dynamics"—and appears successful. It is this ontological order immanent in the structure of the world which thus appears to *define, justify* and *guide* our steps and their proceeding from theory to theory. This order is revealed by the explanation provided in the theories which close over well defined classes of phenomena at each level of the physical knowledge; and by the explanation concerning the progress of physical knowledge where it suggests general principles and regulative ideas and also provides at each step reasons and hints for change.

# 3 Computers in Natural Sciences

## *3.1 Two Moments in the History of Computers*

Historical descriptions are not common in essays, however I think that we should pay respect to the promoters of a development which is practically overrunning us today.

[67] Or "regulative principles"—not to be understood as constitutive (cf. I. Kant, The Critique of Pure Reason, Appendix).

[68] The name "gauge symmetry" is slightly misleading (cf footnote 37), nevertheless this concept proved to be very rich and extremely useful both in developing and in analysing theories.


Charles Babbage (1791-1871) | Ada Augusta Lovelace (1815-1859) | Replica of the Analytical Engine © Science Museum London

**Fig. 4** Two pioneers. From commons.wikimedia.org. Left: Nat Library of Wales Catalog, Public Domain; middle: Science Museum Group, Public Domain; right: CC BY-SA 2.5

The present day developments were already foreseen mid of the nineteenth century. *Charles Babbage*: Mathematician, Philosopher, Inventor, he established together with John Herschel the Analytical Society, later the Royal Astronomical Society. He worked towards dissemination of the Leibniz differential calculus. He was Lucasian Professor of Mathematics (Cambridge), member of the Royal Society and of many Academies of Science. He promoted the British Society for the Advancement of Science. He designed the first programmable, efficient "computer", the "analytical machine", to be used for statistical calculations. Although never built in his lifetime this and further theoretical work is considered as fundamental for the development of computers.

He is often mentioned together with *Ada Augusta Lovelace*, born Byron, considered as "the first programmer". She received private mathematical instruction. She met Babbage as 17 years old and was fascinated by his work to which she kept contact over many years. She wrote programs for the analytic machine, and in 1843 in a paper translating work of Federico Luigi Menabrea (which provided a description of Babbage's analytical machine and programs for it) expressed many original, very interesting ideas, foreseeing among other things the use of computers for symbolic calculations. She denied, however, that computers may develop human-like intelligence (the *"Lovelace objection"*).

About 100 years later we witness the second impulse by which the computer era took its real start. *John von Neumann*, mathematician, physicist, computer scientist, made important contributions in quantum mechanics in formalising the theory and the measurement process, in mathematics, in functional analysis, in logics, in game theory and in computer science where he developed the computer architecture which bears his name. He worked in the Manhattan project to the realisation of the atomic and the hydrogen bomb and supported the concept of assured mutual destruction as the only way to ensure peace in the atomic era. He also devised the idea of self-reproducing automata to be sent in the Galaxy as witnesses of life on the earth.

*Konrad Zuse* (civil engineer, inventor, computer pioneer) devised a number of programmable computers: from the mechanical Z1 (1938) controlled by a perforated film, to Z3 (1941), the first functioning computer in the world, a "Turing complete", i.e. computationally universal machine, working with relays and freely programmable. He built the Z4 (1945), the first commercial computer which was subsequently used for many years at the ETH Zürich. He anticipated programming languages and the *John von Neumann* architecture. He was a passionate painter without having an art study and argued that he did not studied computer science either.

Practically at the same time we witness the work of *Alan Turing*—mathematician, computer scientist, logician, theoretical biologist, cryptoanalyst—who had fundamental influence on computer science. He formalized the concepts of algorithm and computation, devised the so called *universal Turing machine* and provided proofs for computability and for decision problems. In this connection one should also mention the so called *Turing-Church thesis*, which has many variations and interpretations in mathematics, computer science or philosophy. In one formulation the thesis says that physical computability can always be simulated by a Turing machine, which implies digitalisation. It is surely interesting to follow this discussion in connection with *mechanistic explanation;* this also connects directly to the question of the role of mathematics in physics opened in Sect. 2.6., but I shall not touch this here. One of the activities of Turing was building decoding machines which is said to have shortened

John von Neumann (1903-1954) | Konrad Zuse (1910-1995) | Alan Mathison Turing (1912-1954) | Replica of the decoding machine "Bombe" 1944

**Fig. 5** The real start. From commons.wikimedia.org. Left: Attribution; middle-left © CC BY-SA 3.0; middle-right gemeinfrei; right © CC BY-SA 3.0

the war by up to 2 years. He also contradicted the *Lovelace objection* and devised in this connection the well known *"Turing test"* to differentiate between human and machine interlocutors (the tests until now are only slightly positive towards humans).

The ensuing development is dramatic. The "first electronic brain", ENIAC (1945) used vacuum tubes and achieved a speed of about 10 kHz which could be enhanced to 100 kHz or more by parallel processing. A 100 Byte magnetic core memory was added later. It occupied about 60 $m^3$ and needed 150 KW of electric power. A typical laptop today has a speed of about 2 GHz, also to be amplified by parallel processing (about 100,000 times ENIAC), a memory of 1 TByte = 1,000,000,000,000 Byte and a volume of about 1000 $cm^3 = 0.001\ m^3$. It takes less than 15 W of power. Big machines with parallel processing perform by factors of 1000 to 100,000 still better than that. The hardware development triggered software developments and a correspondingly increase of the application fields. Artificial intelligence and robotics start to catch up. This brief history may help to appreciate the future coming upon us.

## *3.2 A View on Computers in Sciences*

*Computers and explanation, Involvement in experiment, theory, understanding; Visualisation*

Before entering the discussion on the role of computers in natural sciences we should remember that computers have long since been involved in epistemological and fundamental questions. We may quote the work of Turing in the foundations of mathematics where he uses the computer paradigm. Later this connection became even more explicit and involved philosophy, driven by the questions of Artificial Intelligence and Cognitive Science,[69] finding its way also in the theory of explanation.[70] This connection was strengthened by the Neural Network paradigm[71] which became the dominant paradigm in the present day Machine Learning field. Since we are interested, however, in the impact of computers on explanation in physics we shall not pursue this direction after having mentioned a few of the big names active here.

1993 the physicist Joseph Dreitlein from the University of Colorado in Boulder published a paper with the title *"The Unreasonable Effectiveness of Computer Physics",*[72] with evident allusion to the 1960 paper of Wigner. He first raises the question, "what are the computers actually doing?" and then starts describing some of their amazingly successful interventions in physics. We shall come back to the first question in the last section. In the following we shall take this (already 27 years old!)

[69] For a few references; Churchland [16], Churchland and Sejnowsk [17], Boden [11].

[70] Thagard [50].

[71] McCulloch and Pitts [38].

[72] Dreitlein [19].

paper as a prompt to illustrate and discuss the present day involvement of computers in physics and the significance of this involvement for the question of explanation.

The role of computers in explanation comes together with the role of calculation in the latter as mentioned in Sect. 2.6. and related to the quantitative—mathematical foundation of physics. We thus find essential computer involvement in experiment and observation, in computer assisted theory development, in finding the right concepts for understanding and explanation. And in all fields and at all stages visualization, data processing, communication, became indispensable tools in research.

Many of these applications involve computer simulation: the computer emulates the dynamics implied by a theory or a theoretical model through the corresponding equations. This is sometimes also called "analysis from first principles" since it only involves the fundamental equations of the theory without appeal to further approximations or simplifying models. Simulations in statistical mechanics and quantum field theory employ furthermore stochastic methods to reproduce the microscopic fluctuations. A brief account on simulations is provided in the Sect. 3.3.

A further development involves symbolic manipulation (already foreseen by Ada Lovelace mid of the nineteenth century): this has been used in many areas and has proven to be essential, for instance in analytic studies using perturbation series (perturbation theory, Feynman graphs) of QFT, in analyses for GRT, in general symbolic programs such as Mathematica and in application from Machine Learning and AI. In the following, however, I shall concentrate on numerical applications in physics. Details and illustrations are given in Sect. 3.2.3.

### 3.2.1 Computer-Assisted Experiment and Observations.

I shall only mention some fields with paradigmatic applications:

(a) *On-line assignment:*

- Astronomical observations today are strongly dependent on eliminating disturbances, so for instance big telescopes work with a system of adjustments of small mirror elements to correct for atmospheric turbulence (adaptive optics). This happens by gauging the image on a known source and performing the corrections and this clearly must proceed in real time.
- High energy collision experiments produce events with tens of thousands of tracks (see Fig. 3 right—compare Fig. 2). One searches for a given signature—as the ones decoded on Fig. 2 (50 years ago this was done by eye …)—and since the events are produced in fractions of seconds one needs to analyse them on-line in real time. This involves extremely fast, sophisticated algorithms for pattern recognition, etc.- besides beam control and general control of the collider. High energy physics experiments are unthinkable without powerful computers and software.

(b) *Calling for precision:*

- Cutting Edge Discovery Science needs high precision and handling of large amount of data. The LIGO experiment, e.g., which in 2015 produced first evidence of gravity waves needs to measure displacements at the level of 1/1000 the size of a proton (~1 fm = $10^{-15}$ m).
- Satellites and space missions, for instance the "New-Horizons" mission which started 2006 following the Voyager 1 and 2 missions and which after reaching Pluto 2015 at a distance of about 5 Lighthours entered the Kuiper belt with flyby of a number of asteroids. 2021 it is proceeding toward the end of the heliosphere aiming to reach the outer space space by 2035 at a distance of about 16 Lighthours (120 AE). The mission includes calculation of the orbit including acceleration near big planets and on board computing for flight control and data management (which clearly must proceed on board, including error detection and reboot, etc.). Its task is to describe and understand the structure of the solar system and its embedding in the interstellar space.

(c) *Empirical enhancement using simulations and impossible perspectives:*

- Milky Way has more than $10^{11}$ stars distributed in the arms of a barred spiral. Our view is from a rather periphery position in the plane of the Galaxy. On the basis of astronomical data computers can, however, help simulating any wanted perspective—see Fig. 6, Sect. 3.2.3a. This helps an intuitive assessment of the situation and of the structure of the Galaxy.
- The computer can simulate effects in the frame of a theory but not observed or even unobservable in nature. Such are problems in celestial mechanics (the design of the flight of space probes, the behaviour of planets and asteroids in "would be" situations—see Sect. 3.2.3b and Fig. 7), or the behaviour of matter at energies and temperature before they are reached experimentally

(a) (b)

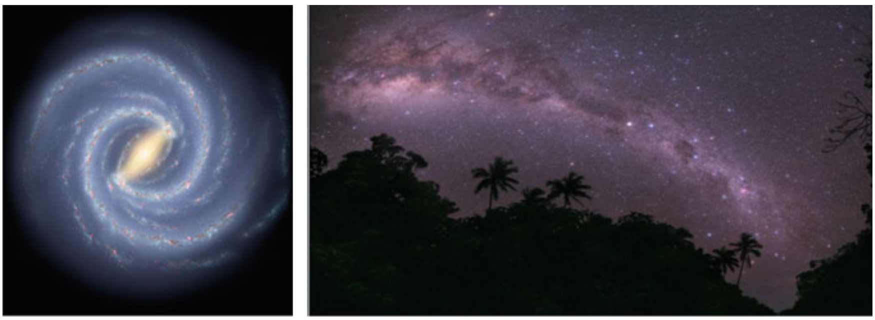

**Fig. 6** **a** View of our Galaxy from above, artist reconstruction using astronomical input (left: NASA.gov, Public) and **b** a real "insider" view of Milky Way on a clear night far from other light sources (above: apod.nasa.gov, MangaiaMW_tezel)

(phase transitions in SM). We can thus obtain data about the predictions of the theory in situations or at parameter values which are not or not yet available experimentally. In cosmology one can simulate not directly observable situations, such as black hole collisions which are sources of gravitational waves, helping the interpretation of real observations or suggesting new effects.

### 3.2.2 Computer Assisted Theory Development

Again I shall only mention a few paradigmatic cases.

(a) *Asking questions and promoting hypotheses (research and curiosity).*

- The non-trivial behaviour of non-linear maps observed in computer simulations (e.g. the Mandelbrot set, the Feigenbaum diagram) led to hypotheses concerning classical chaos. Here visualisation plays a big role—see Sect. 3.2.3c and Fig. 8.
- Non-linear dynamics in complex systems puts many questions for which no analytic solutions can be given. One of the first computer involvements tried to study numerically the question, whether non-linearity ensures ergodicity[73] (*Fermi, Pasta and Ulam, 1953*); what they found was a non-ergodic, unexpected, quasi-linear behaviour. In the sequel of this work very many new insights in the physics of non-linear systems were obtained such as solitons or the interplay of regular and irregular motion, etc.
- Machine learning in the Neural Networks (NN) set up leads to problems which can be defined in the Complex Systems Theory (CS). Here also belongs training NNs for physical applications. One interesting question is whether statistical learning from unspecific reinforcement[74] is possible, that is if the assessment of the actions of an agent and the corresponding reward (positive or negative feedback) concerns not the result of each action but the end result of a series of actions. This is in fact the typical realistic situation in most contexts, think of playing checkers, or of an animal finding the path to water in a forest, or the NN training—the final result counts. We were not only able to answer the question positively but in a neural networks (NN) simulation[75] we also found a very interesting learning flow and an unexpected parameter dependence of the learning behaviour[76] (for details see Sect. 3.2.3d and Fig. 9).

[73] The capacity of a system to take all allowed configurations.

[74] Mlodinov and Stamatescu [39].

[75] Kühn and Stamatescu [35], Kühn et al. (Eds.) [36].

[76] Kühn and Stamatescu [37, 48].

(b) *Promoting and testing hypotheses and models.*

- QCD, the theory of the strong interactions responsible for the formation of nucleons and other *hadrons* from *quarks* and *gluons*, the fundamental fields of the theory, must ensure two important demands: The quarks should behave like non-interacting fields *(asymptotic freedom)* at high energy, while they should be strongly interacting and *confined* in hadrons at lower energy. In a certain representation of QCD belonging to the *Lattice Field Theory* approach (LFT, see Sect. 2.3) the second hypothesis is immanent, while for the first one the support comes from computer simulations.
- Decoding the structure of theories by using models. In LFT models which couple matter and electromagnetic or gluonic fields the effect of the matter fields can be evaluated from summing the contributions from closed paths on the lattice. In a certain example one considers a model accounting for the effect of a background electromagnetic field upon the matter but not for the back reaction of the matter upon the field. It is an example of separating different contributions and using lattice simulation and theoretical results in analysing the theory.[77]

(c) *Deriving post- and predictions from a theory.*

- The building of hadrons in QCD is not amenable to direct analysis and for a while only simple models could be used to obtain, say, the spectrum of hadrons. The development of computer simulations has been able to provide the hadron spectrum and further properties of the hadrons, model-free and without uncontrolled systematic approximations. This has been one of the first big successes of computer simulations in elementary particle physics.
- Besides a low temperature, "hadronic" phase where the quarks are bound in nucleons and other hadrons QCD is also expected to show a high temperature phase, where the hadrons "dissolve" into a "quark-gluon plasma". This theoretical expectation has been tested and supported by computer simulations, before being proven experimentally in high energy collisions at accelerators (at CERN and at the Brookhaven National Laboratory). See Sect. 3.2.3e and Fig. 10.

(d) *Developing and relating theories.*

- We can start with a theory defined at a small length scale (we speak of the UV—*ultraviolet*—scale, short distances). We can ask, what would this theory predict for the phenomena at much larger lengths (smaller energy, IR—*infrared* scale, long distances) and whether we can find concepts in IR and a succinct description for the corresponding phenomena. This is the "renormalization group" approach mentioned in Sect. 2.2 and can be

[77] Schmidt and Stamatescu [47].

followed in both directions: Finding an *effective* description at the IR level from the known UV theory; and developing hypotheses for a UV theory such that the known IR theory ensues. It typically involves further conditions (symmetries, "renormalizability", etc.) to define the searched-for theory. Computer simulations can be employed for both problems.

(e) *Finding the right concepts for understanding and explanation.*

- We mentioned solitons, turbulence, etc. which were studied in computer "experiments". Similar structures are sought in SME *(instantons, vortices)* trying to understand the mechanism of confinement and other expected features of the theory. They have been observed in computer simulations and their role in producing the above effects can be studied there.
- In the NN learning study (see Sect. 3.2.2.a) the peculiar fixed point and separatrix structure found suggests a concept for understanding the mechanisms of learning from unspecific reinforcement (see Sect. 3.2.3d and Fig. 9). The ensued analytic study was prompted by the numerical results.
- The computer simulations for non-linear maps and complex systems have also led to fruitful concepts: self-similarity, fractal structures, hierarchy of scales, etc. which helped understand such phenomena as *classical chaos* and provided thus new instruments for explanation.

### 3.2.3 Visualisation

In all scientific areas computers produce pictorial representations which offer a synthetic grasp of the theoretical structure and connections. Some few examples:

(a) *Impossible views.*

The view of our Galaxy seen from above gives a better intuition than a real picture, Fig. 6.

(b) *Abnormal situations in celestial mechanics.*

The planetary system is considered metastable,[78] but one may ask what could have happened for other initial conditions. In Fig. 7 are shown the orbits around the sun of the earth, the moon (undistinguished from that of the earth at the scale of the picture), and a "lost-mars" which would have been at some time very near to the earth and expelled after a near-encounter toward the left upper corner. This is a simple simulation of Newtonian interaction on a desktop as illustration for the "games" played innumerable times at another scale of precision in conducting planetary missions or controlling the movement of asteroids. The computer simulation allows to change the parameters to produce new effects.

[78] An interesting discussion of the stability properties of the solar system can be found in Petterson [41].

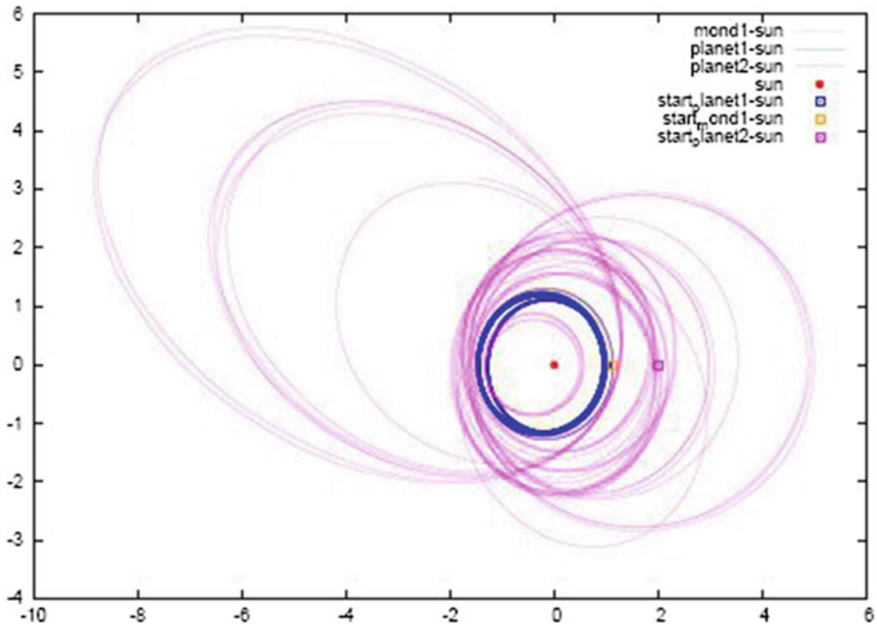


**Fig. 7** 4-body celestial mechanics: m(sun) > > m(earth) > m(mars) > m(moon), ecliptic initial conditions, Newtonian simulation, arbitrary ecliptic coordinates. Orbit and starting point of earth and moon are undistinguishable at the scale of the figure. 

(c) *Classical chaos.*

The Mandelbrot-set $M$ mentioned in Sect. 3.2.2.a is obtained from the non-linear mappingt $z_{n+1} = z_n^2 + c$ in the *complex z plane* and defined as the condition $c \in M$ if the iteration is bounded. The pictures allow an immediate grasp of the peculiar properties of the mapping: fractal structure and self-similarity at different scales, Fig. 8. This mapping is a (complex) deterministic process, but it shows unexpected

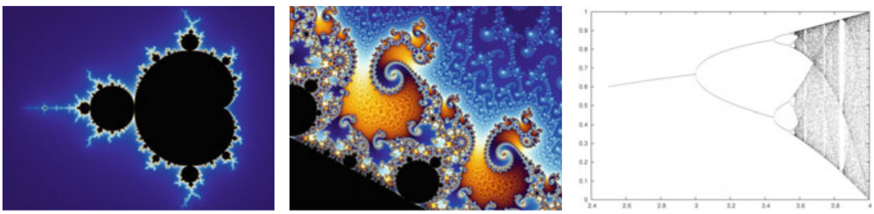

**Fig. 8** *Left and middle*: The Mandelbrot set in the complex c plane and a zoom of a small part of the boundary. Black denotes the areas of convergence, dark blue signals fast divergence, the other colours indicate different speeds in reaching divergent behaviour. From commons.wikimedia.org, CC BY-SA 3.0. Right: The Feigenbaum diagram at given $r$, gemeinfrei, showing the emergence of classical chaos from increasingly rapid bifurcations of trajectories. From commons.wikimedia.org, Gemeinfrei

unstable behaviour which appears nevertheless to generate a complicated, reproducible organization making it a paradigm for "classical chaos". Another approach to classical chaos is described by the bifurcation behaviour of the solutions of the logistic equation $x_{n+1} = r.x_{n.}(1 - x_n), r, x \in \mathbb{R}$ when varying r—the Feigenbaum diagram which shows explicitly the mechanism of chaos generation.

(d) *Learning from unspecific reinforcement.*

In the learning process mentioned in Sect. 3.2.2.a the agent (or "student") is simulated as a neural network. At each trial the student is presented with a series of patterns which he must classify, and uses the so called Hebb rule to modify his internal structure (the *synapses*) according to the *local* stimulus/response *coincidences* between neurons based only upon his up to date knowledge (*blind association* = *self confidence* based on its up to date experience only). The teacher generates the patterns by a fixed stochastic rule and at the end of each trial tells the student which was the *proportion* of the good answers (i.e. in agreement with its—teacher's—own classification). Unless all the answers were correct the student *globally* contradicts *all* previous updates *equally* according to this *global* trial failure (*unspecific reinforcement* = *global feedback*). We called this learning algorithm AR *(association-reinforcement)* and an essential parameter is the strength of the reinforcement, *r* which tells how strong the feedback is compared with the *self-confidence*. Figure 9 shows the flow with the time of the student error $\varepsilon_G$ and the normalization of its synapses *Q* and shows a peculiar structure with various learning curves depending on *r* and separated in two classes. For small values of *r* (lax teacher) the student always learns (the error drops exponentially, right hand curves), but slowly. Increasing *r* (rigorousness) the learning speed improves, but it reaches a threshold $r_0$ above which there is no

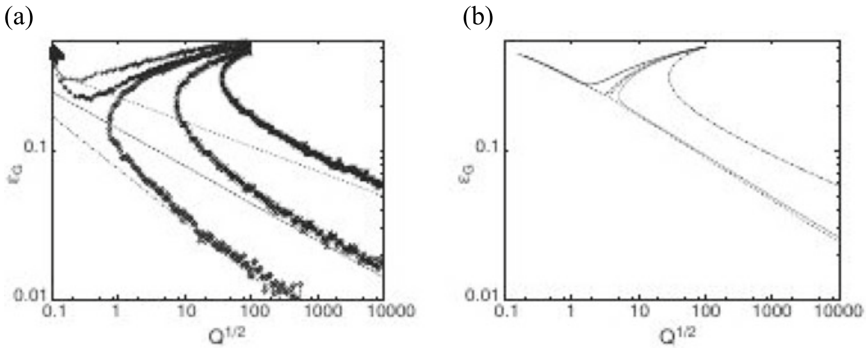


**Fig. 9** Flow with time of the student error in the classification of new patterns (generalization error εG) vs normalisation of its synapses, *Q*. The figures show a flow starting with a candid student (upper middle point) and controlled by an attractive/repulsive fixed point further down which defines a separatrix dividing learning (right hand side flows) from no-learning behaviour (left hand side flows toward the attractive fixed point at εG = 0.5). The curves correspond to increasing rigorousness parameter r from right to left defining on which side of the separatrix the flow will go. The start parameters are slightly different in the two plots. **a** *Left*: computer simulation implementing the AR process. **b** *Right*: exact result from an analytic model representing the AR process. © by the author

learning: the flow turns up toward a fixed point of total confusion in the left upper corner ($\varepsilon_G = 0.5$, the answers are 50/50 guesses). The exponential decrease of the error for $r < r_0$ indicates that the student learned the (unknown to him) rule of the teacher's classification, the fastest for $r$ just below the threshold. All these details are immediately seen from the diagram, Fig. 9. Thus we showed that global, unspecific reinforcement learning is possible, which was our hypothesis but we also obtained an unexpected result that increasing rigour while improving the performance reaches a threshold above which learning is killed. These exciting numerical results prompted an analytic study and in a certain setting the model was found amenable to analytic calculations allowing comparison with the numerical simulations.

A more involved simulation pertains the path of a "robot" on a table with obstacles learning its way to a certain place. It uses again the *association/reinforcement* rule where only the total result of a run is evaluated. A controlled random element in the behaviour of the robot is essential, allowing it to cope with changes or finding better solutions. This model can only be numerically simulated.[79]

(e) *Phase transitions*

The phase transition of QCD mentioned in Sect. 3.2.2.c can also be triggered by populating the vacuum with matter (quarks) which in the formulation of the theory is achieved by introducing a chemical potential $\mu$. The transition can therefore be continued in the plane T—$\mu$ (temperature—chemical potential). The path integral is now genuinely complex which makes the simulation much more difficult. Some of the simulation methods redefine the path integral in the complex plane. The phase transition is signalised by the strong increase of certain quantities averaged over paths (the "order parameters") from practically 0 (cyan) in the hadronic ("confinement") phase to a large non-zero value in the quark-gluon-plasma phase (red). The contour maps of the order parameter describe the behaviour of the transition line in the T—$\mu$ plane and also suggest that the transition becomes sharper with increasing $\mu$. See Fig. 10.

## *3.3 A Brief Account of Simulation in Physics*

Simulation is essentially a computer emulation of physical processes, of their formalisation or of theoretical rules. There are a number of dichotomies applying to this game.

*Concerning the "hardware": Analogue—Digital*

The analogue computer is a physical device using known physical effects. Some early analogue computers used electric circuits and relied on the electrodynamic rules immanent in their functioning to ask and answer questions such as adding exponentials, etc. More involved applications, especially in biology ask how a system

[79] See Stamatescu and Kühn et al. (Eds.) [36].

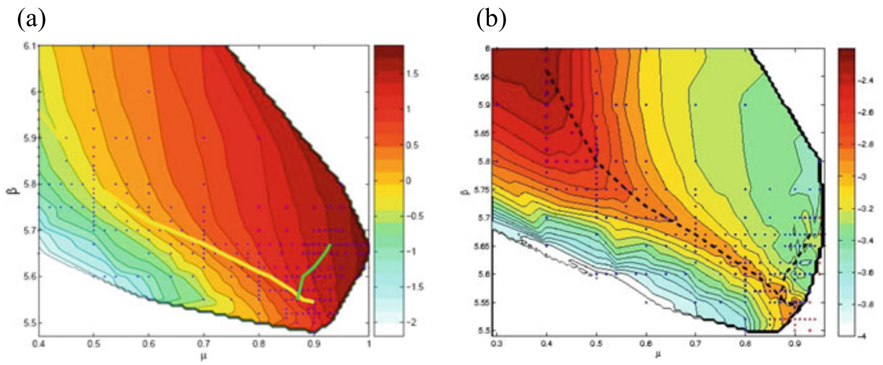


**Fig. 10** Phase diagram of QCD with heavy quarks in the $T\,(\sim 1/\beta\,) - \mu$ plane. **a** *Left*: Order parameter. **b** *Right*: Susceptibility of the order parameter (essentially, its slope across the ridge) showing clearly the transition line. © by the author

of interconnected cells subject to an initial perturbation would behave as a whole: smooth, oscillatory, abrupt, etc. under varying the parameters of the system (e.g., the connections between the cells or the temperature). Hybrid analogue–digital systems use electronic models for the cells—so for neuron assemblies the so called Hodgkin-Huxley neuron realised with electric circuits and represented as a set of differential equations—to simulate the activity of biological neuron networks (see also Sect. 2.4).

The present day landscape is, however, dominated by the digital computer, whose history was hinted at in Sect. 3.1. Its involvement implicitly assumes that all our "encounters" with nature can be analysed in terms of human (binary) logics[80] (an instance of the Turing-Church thesis). Digital computers use rational numbers and binary operations to perform every real number operation. A digital computer can also be represented as a neural network (a network of artificial binary cells) and following the celebrated Charles Sherrington remark that "what the brain does is to take decisions" as taken over by McCulloch and Pitts[81] to introduce the neural networks, we appear to having closed the circle relating digital computers with human logics. Neuroscience and many directions in Artificial Intelligence followed this line and we witness a very rapid development.

Every knowledge which can be formalized can be implemented on digital computers (as already foreseen by Ada Lovelace mid of the nineteenth century and formally developed by Alan Turing 100 years later). Digital computers are of course "classical" devices, but they can also simulate quantum theory by implementing the corresponding rules *(Schrödinger equation, measurement rules,* etc.*)*. Notice that this is not what the quantum computers do: the latter do not simulate the theory but

[80] Non-standard logics can also be represented in binary logic.

[81] McCulloch and Pitts [38].

implement the phenomenon itself and use the theory for designing the system and interpreting the results.[82]

A simulation is an algorithm following a number of rules to produce at each step a set of values for the variables representing the basic quantities describing the analysed system (a "configuration"). The rules are designed according to the problem at hand. The configurations are then used to obtain solutions to the problem as limits or averages of the relevant quantities ("observables").

*Concerning the algorithm: Deterministic—Stochastic*

While the deterministic algorithms calculate at each step exactly (at the level of the machine precision) the new values of the variables in accordance with the equations of the theory, stochastic algorithms introduce a controlled random element ("noise") in their procedure which now involves "stochastic" variables. The noise is usually meant to take into account the physical fluctuations for instance in statistical or in quantum physics and it is represented in computation as "pseudo-random numbers" generated by some mathematical routine. There are different types of stochastic processes: non-linear or linear (the noise does or does not depend on the variables), Markovian or non-Markovian (each step depends only on the previous variable's configuration or on the whole preceding history), etc.

*Concerning the problem set up: Classical—Quantum*

Classical problems involve, for instance: Simple iterations such as the one described in Sect. 3.2.3c (the computation is simple but it needs to be repeated billions of times); Solving systems of differential equations, such as in Sect. 3.2.3b. Both use deterministic algorithms. Also implementing learning rules for evolving a neural network as in Sect. 3.2.3d is a classical problem, but it may use a stochastic algorithm to introduce uncertainties in behaviour of the learner (agent).

Simulations of classical statistical mechanics systems at equilibrium also use stochastic processes to produce statistical *ensembles*. One proceeds from the so-called *partition function* whose expression describes the ensemble of configurations with their weights—the Boltzmann factors, which are positive definite and can be interpreted as probabilities. Since the number of configurations (i.e., situations of the system) may be enormous the algorithms performs "importance sampling" according to these probabilities using a *real stochastic process*. The collection of configurations so obtained is then used to obtain averages of interesting quantities, study phase transitions, etc.

Also simulations in quantum physics use stochastic algorithms to produce ensembles of configuration. A typical quantum theoretical problem is *Quantum Chromodynamics* (QCD), a quantum field theory, see Sect. 3.2.3e. Here we start from the path integral formulation in which, however, the weights of the paths are now complex

[82] There are a number of approaches in this field which mix analogue (cold atoms, optical lattices, etc.) and digital features in various combinations.

and cannot be used as probabilities for importance sampling. The trick is to use certain mathematical features of these theories which allow to rotate the time in the complex plane from the real to the imaginary axis (*Wick rotation*). In a second step we *discretize* the fields on a space-(imaginary) time lattice. We obtain in this way a so called *Euclidean Lattice Field Theory* (LFT) which is essentially a *Statistical Mechanics* system at equilibrium with real, positive Boltzmann factors and for which we can use the same methods as above. In the end we must interpret the results back in real time.

However even in the Euclidean formulation some physical question, such as unbalanced background charges introduce imaginary parts in the action. Moreover, there are problems such as non-equilibrium dynamics which require real time evolution and must be studied on a Minkowski lattice without performing the Wick rotation. In such cases refined algorithms are called for since the Boltzmann factors are now complex. The most studied procedure is to redefine the variables as complex numbers and extend the analysis to their complex planes. A far developed approach which has provided results for realistic situation (e.g., QCD for non-zero baryon density) uses a *complex stochastic algorithm*, the Complex Langevin Equation.[83]

As can be seen, simulations build up a domain for themselves. This includes setting up the theory in an adequate form, developing algorithms, etc.[84] These studies are called "from first principles" since they directly implement the basic relations of the theory. The role of simulations is to ensure computability for complex theories which is one major factor in explanation. Besides producing post- and predictions for empirical tests of the theories (*deductive effort)* they also hint at many *right concepts* and lead to insights into the theory and contribute to the *abductive effort* by suggesting and testing hypotheses. Simulations are very important in evolving explanation as related to the particular theories as well as to their progress. With the rapid development of the computers we may generally expect synergy effects between application and theoretical development in computer science with further impact on sciences.

## *3.4 The New Computing*

*Machine learning; Neuromorphic computing; Quantum computer; Entanglement and decoherence*

The tremendous development in both hard- and software has opened the way for a new definition of the role of computers in science. Here a brief account of the present day involvement of computers should be provided: the new computing. This regards both the hardware and the tasks and methods. The main features of this development can be subsumed in three notions: miniature and flexible design, neural networks

[83] Cf. Scherzer et al. [46] and references therein. For a review see Berger et al. [6].

[84] Of course one uses simulations also for processes, hypotheses, etc. as far as these can be formalized.

and complex architectures, machine learning and autonomous development. Many present approaches are expanding research from the end of the last century; it is, however, its present momentum in opening new perspectives and applications which may justify the term "new computing".

For an example, I shall briefly mention one comprehensive program which shows many of the present lines of research: the European Human Brain Project (https://www.humanbrainproject.eu). As already the title suggests, the program has a strong connection to human biology and cognition. It is distributed over many research groups. It involves fundamental and applicative research and is set up to provide interactions and synergy effects at various scales concerning.

> Neuroinformatics: Brain atlas, data sets, 2D-3D viewer,
>
> Brain Simulation: Simulation of neurons and collectives, validate models,
>
> Analysis of high level brain functions: *From pattern recognition to cognition,*
>
> High Performance Analytics and Computing: Large scale data mining, large scale simulations,
>
> Medical Informatics: Bridge brain-science, clinical research and patient, improve diagnosis,
>
> Neuromorphic Computing: Simulations on special architectures inspired from biological brains,
>
> Neurorobotics: Link simulated brain to robotic bodies, test brain and robot models,
>
> Ethical and Societal Assessment: Accompanying studies and discussion,

with influence from and upon related areas including machine learning and physics simulations. Just for an impression, brain models have been developed at the scale of a rodent brain, and tests for brain function models on neuromorphic computers allow a speed up by a factor of 1000 over biological processes.[85] The Human Brain Project above gives an impression on the horizon of the present developments.

A recent development which is interesting also for the question of explanation takes place in the frame of simulations for systems with many degrees of freedoms, which include QFT defined as LFT (see Sect. 3.3). Such models typically show phase transitions, see e.g. Sects. 3.2.2c and 3.2.3e which we can observe in computer simulations and describe using *order parameters*—observables distinguishing between the different phases. This behaviour is visible in the configurations produced in the simulation and the order parameter is in most cases suggested theoretically. In that sense the computer helps *testing* a hypothesis. Models with a more complicated structure may show more phase transitions and the building of hypotheses for *order parameters* may be ambiguous. Using machine learning methods in a refined neural networks set-up and an adequate way of "asking" the computer may itself *propose* a hypothesis and may provide access to the "*right concepts*", represented here by the order parameters. Such methods are also used in data mining, pattern finding,

[85] Wunderlich et al. [56] and further publication of the Neuromorphic Computer Group at the University of Heidelberg. Neuromorphic computers are "hybride" (analog-digital) machines with some millions of Hodkgin-Huxley neurons in variable architectures.

etc. This is an example of how computer science (here: *machine learning*) enters the problem of explanation in physics beyond calculation and simulation.[86]

The above examples concern classical computers. A rapid development presently pertains also quantum computers[87] which in some sense and to various degrees can be seen as analogue computers. By now their development followed the classical binary paradigm with the equivalent of the neurons being here two-states quantum objects (qubits) which could be brought in entangled states. Equivalents of the logical gates *(and, or, not,..)* are then defined and as long as we can shield the systems from *decoherence* effects due to the environment we can use the *entanglement* in specially designed algorithms for non-classical calculations. The effort until now has been to show that q-computers can outperform classical ones on some selected problems such as factorization large integers (interesting for cryptography) where the corresponding algorithms for classical computers would be much less efficient. The general superiority is still under debate. But further developments which would take advantage of the full quantum zoo could open new horizons. This may affect the full architecture—e.g., by redefining the "qubits" on higher complex manifolds and re-designing the "logical gates" accordingly—definitely breaking with the classical paradigm. Genuine analogue quantum simulation may represent a far reaching perspective leading to unforeseeable developments both in applications and in connection with explanation.

## *3.5 What Are Computers Actually Doing?*

We have seen computers being involved in essential ways in practically all domains of physics research in all fields. They help or permit performing and interpreting evolved experiments, they allow extrapolating our empirical basis beyond its natural limits. They are involved at all stages of theoretical developments: inductive, in data handling, deductive, in obtaining post- and predictions from the theory, abductive, suggesting hypotheses by producing unexpected effects. In the fields of the fundamental interactions, of complex systems, of astronomy and cosmology, etc. Thereby computer simulations became a powerful tool in all these enterprises. So what can we say about the computers commitment in explanation?

Dreitlein [19] quotes two typical points of view of scientists concerning the involvement of computers in science. Computers can be seen as:

- producing final data from initial data according to some given rules, or
- reproducing the "code of nature".

Concerning the first perspective we must remember that computers are *not supposed to produce new physics,* but they can help us understanding the hints from nature by helping us to obtain empirical information and by bringing us on the track

[86] For an introduction and review see Carleo et al. [14].

[87] For partial assessments see e.g. Altman et al. [1], Grambling and Horowitz [26].

of effects inherent but hidden in the observational data. Moreover, the computers also directly support explanation by allowing to test our theories and "decode" them and find or suggest relevant concepts. And computers help us at an important step in the theory development by allowing to test and develop hypotheses on the way to new or improved explanation.

Hence: *Computers, while not directly explaining nature, provide vital knowledge and tools for explanation, assisting the scientist in an interactive game in his work to explain the world.*

But we don't know what the future developments, e.g. in Artificial Intelligence will bring (may *Turing's* refutation of *Lovelace'* objection hold?), and whether in a (far?) future computers may be able to learn more about the universe than we do … And this brings us to the second perspective. This is of course a speculation, nevertheless let us see what it might mean:

– In a trivial sense it just says that computers reproduce our logical thinking, which is (at least partially?) compatible with nature since it may have been shaped by the history of our interaction with the world; thus computers help us extend our logical capacities (see Sect. 3.3).
– But in a less trivial interpretation it says that *computers may help us overcome the limitations of our classical logical thinking and access new thinking horizons* (may *quantum computing* be a suggestion in this direction?) bringing also *new dimensions* in explanation.

Whatever the answer, we may expect a lot of development—and fast.

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