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Introduction: Computer Simulations as a Complement to Quantum Theory?

In this paper I will provide some historical perspectives on the question at the core of this workshop, namely the many ways in which computer simulations may be contributing to reshape science in general and quantum physics in particular. More specifically, I would like to focus on the issue of whether computer simulations may be regarded as offering an alternative, or perhaps a complementary, version of quantum theory. I will not be looking at the way in which computer simulations are used in quantum physics today, since this task has been outstandingly fulfilled by other contributions to this workshop. Instead, I will present a few episodes from the history of quantum theory in such a way as to make it plausible that simulations might indeed provide the next phase of historical development.

In what sense can computer simulations be regarded as "theories," though? How can a computer simulation be on a par with the Schrödinger equation of quantum mechanics? To answer this question I will start by discussing (and criticizing) the rather naïve, but very widespread ideal of "theory" that dominates much of today's fundamental physical research, and of which quantum mechanics constitutes a paradigmatic example.

There is little doubt that quantum mechanics is seen today as an epistemically privileged physical-mathematical construct, and this status is hardly surprising, because quantum mechanics provides the basis for a large number of experimentally successful quantitative predictions. However, the predictive efficacy is by far not the only factor supporting the authority of quantum mechanics. Of paramount importance is the fact that it conforms to an ideal of theory that emerged in the course of the nineteenth century and still largely dominates physical research today: a "theory" as a coherent, rigorous mathematical construct expressed in symbolic formulas from which testable numerical predictions can (at least in principle) be derived. Such a construct may then be coupled to a physical interpretation expressed in verbal terms, to deliver not only predictions, but also explanations of phenomena. As I have discussed at length in other publications (Borrelli 2012; 2015a; 2015b), this image of a physical-mathematical construct both numerically predicting and verbally explaining phenomena is a fundamental template of authority in the physical sciences (and often also beyond them), despite the fact that not even long-established "theories" such as classical mechanics or electromagnetism actually conform to it.

Few, if any, mathematical theories can remain coherent and rigorous if they also have to provide procedures for actually computing predictions. Even in those very rare cases in which an equation like Schrödinger's can be solved exactly, applying the solution to a real-world case always requires adjusting it in some way that will make it not any more coherent with the original equation. In quantum mechanics the connection of Schrödinger's equation with phenomena is particularly problematic, because in the standard Copenhagen interpretation the measurement process is assumed to irreversibly change the state of the quantum system. During a measurement, in the standard interpretation, a so-called reduction of the wave function occurs: the wave function associated with the quantum state immediately before the measurement is instantaneously replaced by a different one that reflects the outcome of the measurement.[1] In other words, there is no coherent mathematical structure capable of modeling the process of measurement in a quantum system.

1 On the Copenhagen interpretation of quantum mechanics, the measurement problem and the alternative interpretations proposed since the 1950s (see Faye 2014). It is not my intention to discuss here interpretative issues of quantum mechanics, since no satisfactory solution for the measurement problem has been found so far, and the Copenhagen interpretation remains the dominating one, at least among practicing physicists.

In general, the image of a theory as a rigorous and coherent mathematical construct from which numerical predictions can be derived has little or no correspondence in actual research. Yet this image still dominates science and endows constructs like the Schrödinger equation with a special authority. A key feature of this special status is that, both in today's scientific culture and in the popular imagination, symbolic formulas are usually regarded as mere vehicles to convey abstract, disembodied conceptual structures whose features are fully independent from the form in which they are expressed.

In contrast to this view of theoretical knowledge, I believe that theories are "abstract" only in the sense of being far removed from everyday experience, not in the sense of being "disembodied." Science is first and foremost a collective enterprise, and so no theory can exist that is not expressed, communicated, and appropriated by means of some aesthetically perceivable form, such as symbols, words, diagrams, three-dimensional models—and perhaps also computer simulations. Mathematical symbols, for example, are obviously visual and, for those who are familiar with the rules for manipulating them, they also possess a haptic component (Borrelli 2010; Krämer et al. 2012; Velminski and Werner 2010). This material and performative dimension of theories does not allow a sharp separation of form and content and is an essential factor shaping their employment in research practices. To put it in other terms, I would like to claim that the dynamics of medium and message apply also to physical theories.

Therefore I will now discuss some episodes from the history of quantum theory by highlighting the role of the material, performative dimension. I will show how, in the early days of quantum theory, the range of forms mediating theories was much broader than one might expect. I will argue that, if we set aside the ideal of theory as a disembodied construct necessarily manifesting itself only in rigorous mathematical formulas, there is little difficulty in considering computer simulations as a medium of quantum theory on a par with the many symbolic and diagrammatic constructs that were developed in the pioneering years of the discipline.

Spectroscopy between Arithmetics and Geometry

I begin my overview by considering what is today referred to as "classical physics", that is, the many theories developed or refined over the course of the nineteenth century, such as mechanics, electromagnetism, acoustics or hydrodynamics. In that context, there was one medium of theory enjoying a very privileged status: differential equations and the functions solving them. Differential equations worked very well in delivering numerical predictions for a wide range of phenomena, but some areas appeared problematic. The experimental field that most decisively contributed to the rise of quantum theory was the study of light and its properties, and more precisely the phenomena of spectral lines and black-body radiation. It was in those contexts that refined differential equations came to be replaced by very simple arithmetic formulas as the most effective medium to theoretically capture observation.

Already in the early modern period it had been accepted that white light resulted from a superposition of colored rays, and when in the nineteenth century the wave theory of light became established, each colored ray that could not be further decomposed came to be associated with a wave of specific length and frequency. Around 1850 physicists noticed that the light produced by igniting different chemical elements was made out of different, discrete sets of colors (i.e., wavelengths).[2] By the late nineteenth century physicists had developed a new research object: "line spectra," that is, the sets of lines produced by decomposing the light emitted by various substances.

[Fig. 1] Line spectrum of hydrogen (Source: Huggins 1880, 577).

Line spectra such as the one of hydrogen shown in Fig. 1 clearly displayed a discontinuous character, with each element emitting light only of specific, discrete wavelengths, whose numerical values could be estimated by measuring the distance between the lines in the spectrum. The discontinuity of spectra was problematic because if microphysics was ruled by differential equations having smooth, continuous solutions, then the light emitted should have formed a continuous spectrum—not a discrete one.

Researchers at the time made various proposals for how to connect the experimental results with available theory. One approach often employed was to make an analogy between light spectra and acoustic vibrations,

2 The following overview of the development of spectroscopy and of spectral formula is based on Hentschel (2002). For the role of spectroscopy in the development of quantum theory see Jammer (1966).

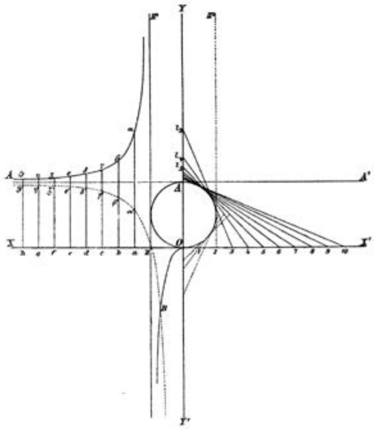
which had been successfully represented in mathematical form through the so-called harmonics (i.e., Fourier series of sine and cosine functions). However, such approaches were not very fruitful, and the breakthrough occurred only with the proposal of Johann Jakob Balmer (1825–1898), who was not a physicist, but a mathematician and an architect, and in particular an expert in the field of architectural perspective drawing. Never having worked on spectroscopy before, Balmer in 1885 published a short paper in which he proposed that the wavelengths of the hydrogen spectral lines would conform to the very simple formula:

$$\mathrm{H}(m, n) = h\frac{m^2}{m^2 + n^2}$$

with H the value of a given wavelength, (m, n) two integer numbers and h = 3,645 a constant computed on the basis of measurement (Balmer 1885, 81, 83). For m = 3, 4 and n = 2 Balmer's formula fit very well the measurements available, and in the following years it turned out that also for higher values of m and n the formula matched the wavelengths of newly observed hydrogen lines.

How did Balmer, a mathematician and architect who had never shown an interest in physics, arrive at his formula? We have no direct sources on this issue, but historian and philosopher of science Klaus Hentschel has offered a very plausible answer based on an analysis of Balmer's work and of archival material (Hentschel (2002, 295–301, 442–448; Hentschel 2008). In his 1885 paper Balmer did not explain how he had arrived at his formula, but some years later, in 1897, he again wrote about spectroscopy and showed how an improved expression could be derived based on a geometrical construction similar to those employed in architectural perspective drawing, in which Balmer was an expert (Balmer 1897). In his 1897 paper Balmer explained that the hydrogen wavelengths could be constructed geometrically as shown in the right half of Fig. 2.

First one should draw a circle whose diameter AO represents the minimum wavelength of hydrogen. Then the points 1, 2, 3... are drawn along the X-axis at equal distance from each other. By drawing the tangents to the circle passing from points 3, 4, ... and looking where they intersect the vertical axis, one obtains the wavelengths of the hydrogen spectrum as the distances between point O and the intersection points. This construction is the same as that employed to derive the perspective shortening of a circular column as seen by an observer walking along the X-axis and pausing to look at the column at points 3, 4 ...



[Fig. 2] Geometrical derivation of spectroscopic formula (Source: Balmer 1897, plate VIII).

Hentschel argues that this geometrical derivation was similar to the way in which Balmer came to his formula in the first place: his experience with perspective drawing led him to visually perceive the spectral lines in terms of a familiar construction for the shortening of a fluted column. It is not possible for me to present here Hentschel's detailed argument, but an important point he makes is that while physicists at the time focused on an analogy between light and sound that was expressed in terms of frequencies and mathematical functions (harmonics), Balmer worked visually and geometrically, and so could open up new paths of reflection. Here we see an example of how the employment of different media to express the "same" knowledge could lead research in diverging directions. For us today Balmer's symbolic formula represents a physically significant result, which prompted the development of quantum theory, while his geometrical reasoning appears to be purely contingent. Yet Balmer saw geometrical methods as a significant guideline in research and, after describing the geometrical construction in Fig. 2, he stated:

> This construction may possibly be useful in throwing a new light on the mysterious phenomena of spectral lines, and in leading to the right way of finding the real closed formula for spectral wavelengths, in case it has not already been found in the formula of Rydberg. (Balmer 1897, 209)

Balmer's rule for deriving hydrogen spectral wavelengths could be expressed both in arithmetical and geometrical terms, but the choice of medium had epistemic implications. Balmer's contemporaries, perhaps unsurprisingly, chose the arithmetic formulation, and today the idea of using geometrical construction for theoretical guidelines may appear very far-fetched. Yet it was probably geometrical reasoning that produced Balmer's formula in the first place and, as we will presently see, theorists later developing quantum theory did not shy away from very far-fetched constructions expressed in symbolic notation.

By the early twentieth century Balmer's formula had been developed into more general expressions for spectral series, according to which all frequencies of light emitted by atoms could be expressed arithmetically as the difference between two terms, each depending on a positive integer (m, n), on the universal "Rydberg constant" R, and on a number of other constants (s, p, d...) depending on the kind of atom.[3] The formula looked like this:

$$\nu(m, n) = \frac{R}{(n + s)^2} - \frac{R}{(m + p)^2}$$

Such simple formulas could fit practically all the results of atomic spectroscopy, a rapidly expanding experimental field at the time. By finding the values of the constants s, p etc. on the basis of the first few lines in a series, predictions for lines with higher m, n could be obtained, and they often turned out to be correct. The fact that the formulas were based on integer numbers seemed at first surprising, and some authors at the time tried to find a differential equation from which such formulas could be derived, but in this early phase the search was to no avail (Hentschel 2012). For more than a decade, the formulas for line spectra resisted all attempts to embed them in an overarching physical-mathematical framework, or at least provide them with a verbal interpretation with explanatory character. The formulas remained what I would like to characterize as "mathematical fragments," that is, physical-mathematical expressions which, although complete in themselves, stood in isolation from the theoretical landscape of their time. Theorists used them as starting points to try and construct broader theoretical frameworks, treating them as though they might be traces, "fragments" of a (hypothetical) overarching theory that had yet to be formulated.

3 The information contained in the following overview on the development of quantum mechanics can be found for example in Jammer (1966). On the role of series formulas in the development of quantum theory see also Borrelli (2009; 2010).

In the early twentieth century spectral series were not the only "mathematical fragments" involving natural numbers that played a role in microphysics: there was also Planck's formula for black-body radiation. Like Balmer's formula, Planck's expression had been derived bottom-up by matching experimental results in a situation where all top-down derivations from electromagnetic theory had failed to provide empirically plausible predictions.[4] Planck's formula could be seen as implying that the energy exchange between matter and electromagnetic radiation could only take place in finite quantities, and that the minimum amount ("quantum") of energy exchanged by matter with light of frequency ν was $h\nu$, where h was Planck's constant.

Bohr's Atom and the Old Quantum Theory as Multimedial Constructs

By the early twentieth century simple arithmetic formulas involving positive integer numbers had taken center stage in the search for a theory of "quantum" physics, and in 1913 the Danish theorist Niels Bohr (1885–1962) combined them with elements from classical physics and verbally formulated physical assumptions to produce "Bohr's atom," a very innovative theoretical construct.[5]

First of all Bohr assumed that the hydrogen atom could be regarded as a small solar system governed by a classical differential equation defining its possible orbits. Then he introduced a novel physical principle expressed verbally: only those orbits having certain particular values of the energy were actually realized, because only in them would the atom not radiate and would thus remained stable.[6] These stable orbits were called "stationary states" and, according to Bohr, radiation only occurred when the atom "jumped" from one stationary state to another. The energy E lost (or gained) by the atom corresponded to the creation (or annihilation) of light of frequency ν such that $E = h\nu$, as required by Planck's formula. Each of the stationary energy levels was linked to an integer number, chosen so as to exactly match one of the two terms in the hydrogen series formula.

4 The history of the emergence and transformation of Planck's black-body formula has been studied in much detail by many historians and cannot be discussed here. A recent overview with further references is Badino (2015).

5 For a recent, exhaustive treatment of Bohr's atomic model and its development see Kragh (2012).

6 The stability of matter was a problem for the solar system atom in classical physics, since in classical electromagnetism a moving electron would radiate, lose energy, and eventually fall into the nucleus.

Since all spectral series formulas were differences between two similar terms, they could all be interpreted as expressing the difference between the initial and final energy of an atom. Clearly, the predictive value of Bohr's atom was identical to that of the spectral formulas on which it was based, so no new knowledge was actually obtained. However, now the "mathematical fragments" were connected to a more complex construct that involved both classical orbits and novel notions like "stationary states" and "quantum jumps"—a construct that is regarded as the first quantum theory, combining functions, arithmetic formulas, and verbal statements in what may be characterized as a multimedial whole. The fact that verbal statements played such a crucial role in Bohr's atom was typical of his work, and it is no accident that he is often highlighted as one of the most philosophical scientists of his time. Despite its hybrid, innovative character Bohr's atom was very positively received, and soon became the core of what is today known as the "old" quantum theory, which was developed between 1913 and 1925 by Bohr himself, and by many other authors.[7]

In the "old quantum theory" each possible stationary state of an atom was associated with a set of integer (or semi-integer) numbers derived by performing an increasing number of spectroscopic measurements, and then fitting these empirical results with spectral formulas containing the quantum numbers of the various stationary states. Although these sets of "quantum numbers" may appear to be nothing but a group of natural numbers, they actually constituted a new form of theoretical representation—a new medium of physical theory that was necessary to represent and manipulate the new notion of "stationary state." In principle, each stationary state was also associated with a classical orbit but, as the formal intricacy of the theory increased, quantum numbers became more and more the primary means to aesthetically represent and manipulate the innovative, and in many ways obscure, notion of stationary state introduced by Bohr.

Physical Quantities as Infinite Matrices

By 1925 quantum theory had proved to be capable of subsuming a large number of new experimental results in spectroscopy, but it still remained an extremely fragmentary construct that physicists kept on modifying and enlarging to accommodate new spectroscopic evidence. Scientists involved in this task usually justified their modus operandi by invoking Bohr's

7 For details of these developments see for example Kragh (2012), Jammer (1966), or Borrelli (2009).

"correspondence principle," a very flexible—not to say vague—heuristic tool to formally derive quantum relationships from classical ones. In 1925 the young physicist Werner Heisenberg (1901–1976) made a proposal for a new way of reframing and unifying the results obtained up to then, and further developed his suggestion together with Max Born (1882–1970) and Pascual Jordan (1902–1980).[8] The result of this process was "matrix mechanics," a theoretical construct perhaps even more innovative than Bohr's atom. Matrix mechanics was a theory expressed in part in verbal terms and in part through symbolic expressions, which although at first sight appeared to be mathematical structures in fact did not correspond with any rigorous, coherent objects of the mathematics of their time.

Matrix mechanics emerged quite rapidly over the course of a few months during 1925, but the process of its construction was extremely complex, and I will not attempt to summarize it. I will instead offer a brief overview of the new theory, arguing that it represented not only a fundamental step from a physical point of view, but also a further radical transformation of the way in which "quantum theories" were aesthetically made available to fellow scientists.

Just as was the case for Bohr's atom, matrix mechanics did not bring with it new testable predictions, but rather offered a different, more unitary set of rules for obtaining already known results. Matrix mechanics took over the key new elements from the old quantum theory: the idea of stationary states associated with sets of quantum numbers and that of quantum jumps from one state to another. Classical orbits were left out: Heisenberg explained that physics should only deal with "observables," and in atoms the only observable quantities are the frequencies and intensities of spectral lines, which are not linked to a single electron orbit but to the transition between the two of them. The exact position and velocity of an electron orbiting around the nucleus, on the other hand, are not observable and so should have no place in quantum theory. Heisenberg's key original idea was that quantum-physical quantities should not be theoretically conceived and represented as having at each instant a single numerical value, as was the case in classical physics, but rather thought of as always related to an infinite set of values. Accordingly, each physical quantity was associated with a set of infinitely many values, which were ordered into a two-dimensional matrix having infinitely many rows and columns. In the case of the hydrogen atom each row and each column was labeled by the quantum numbers of one hydrogen stationary state, as is seen in the formula below,

8 For an overview on the emergence of matrix mechanics see Jammer (1966, 196–220).

where “n” and “m” stand for one or more quantum numbers describing a stationary state.

$$\begin{bmatrix} M_{1,1} & M_{1,2} & \dots & M_{1,m} & \dots \\ \dots & \dots & \dots & \dots & \dots \\ M_{n,1} & \dots & \dots & M_{n,m} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix}$$

In this way, each element of the matrix was formally linked to a transition between two atomic states, providing a fitting scheme to express the observable values of frequency and intensity of atomic radiation. Born, Heisenberg, and Jordan stated the rules for how to construct the matrices and manipulate them to obtain spectroscopic predictions. The details of this procedure are not important for the subject dealt with in this paper, but it is very relevant to note that these “infinite matrices” were no rigorous mathematical constructs. Born, Heisenberg, and Jordan manipulated them according to the usual rules for adding or multiplying finite matrices, but they fully acknowledged that for infinite matrices those rules led to infinite sums, which in all probability did not converge. For their aims it was sufficient that the physically relevant results obtained would make sense. In other words, the infinite matrices were a new medium of quantum theoretical practice through which predictions could be obtained.

In late 1925 Born collaborated with the already renowned mathematician Norbert Wiener (1894–1964) to generalize the formalism of matrix mechanics into “operator mechanics,” which would be both physically significant and mathematically rigorous. However, their attempts were soon preempted by the unexpected appearance in early 1926 of Erwin Schrödinger’s (1887–1961) wave mechanics.

The Return of Differential Equations

As we have seen, the development of quantum theory had taken a path that led it further and further away from the differential equations that dominated classical physics. With matrix mechanics and Heisenberg’s suggestion of discarding atomic orbits, the formal development had also produced quite radical physical interpretations. However, differential equations made a surprising reentry into the game with a series of papers published by Schrödinger in the space of a few months in 1926.[9] Schrödinger had found an exactly solvable differential equation whose solutions $\psi_{m, n, l}$ depended on a set of three integer and semi-integer parameters (m, n, l) which precisely coincided with the quantum numbers of the stationary states of hydrogen. This was an essential new development as far as predictive power was concerned: both in the old quantum theory and in matrix mechanics quantum numbers had to be derived from empirically based spectroscopic formulas like Balmer's and then inserted by hand into the theory. Schrödinger's equation instead allowed the derivation of hydrogen quantum numbers without making reference to experiment. Similar equations could be written for all atoms and, although they could not be exactly solved, one assumed that they would in principle allow the derivation of the energy levels of the atoms. In a sense, Schrödinger's equation was a very complex and redundant apparatus to derive quantum numbers, and the question now was how its many parts could or should be interpreted physically. It was a new medium of theory opening up a huge new space of physical-mathematical speculation.

Schrödinger was understandably convinced that atomic spectroscopy might be reformulated in terms of the functions $\psi_{m, n, l}$, which he interpreted as describing "matter waves." However, the Schrödinger equation by itself could not deliver any spectroscopic prediction, as one still had to assume that quantum numbers corresponded with stationary states, and that "quantum jumps" between states would lead to radiation. As is well known, Schrödinger made it his main task to get rid of quantum jumps by appropriately extending his theory, but was never able to do so.

By 1927 the refined, if somehow still fragmentary, theoretical apparatus of quantum mechanics was in place, and it comprised Schrödinger's equations and their solutions, infinite matrices, and a verbally expressed statement about "quantum jumps" between "stationary states," which had originally been introduced by Bohr. The interpretation of the new theory was still quite fluid, and some features of Schrödinger's equations provided material for discussion.

A very important feature of the equation was the fact that if two functions solved it, then any linear combination of the two would be a solution, too. If a combination of two stationary states was also a solution, did this mean that an atom could be in two stationary states at the same time? Schrödinger had no problem with this view, since for him the "states"

9 For an overview of the early development of wave mechanics see Jammer (1966, 236–280).

were nothing but waves in a "matter field," and two waves could always be superimposed. Other authors however disagreed, among them Born, who suggested that the quantum wave should be interpreted as giving the probability with which an atom was in one or another state: "an atomic system can only ever be in a stationary state [...] but in general at a given moment we will only know that [...] there is a certain probability that the atom is in the n-th stationary state" (Born 1927, 171).[10]

This was an early statement about the "statistical interpretation" of quantum mechanics, and it marked the start of discussions on whether the idea of wave-particle duality that had been assumed for light quanta (i.e., photons) could and should also be regarded as valid for electrons and protons.[11] We see here how the (re)introduction of the classical medium of theory, differential equations, and function led to new physical questions. These in turn prompted scientists to further analyze quantum mechanics, both by trying to reframe it into more rigorous, unitary mathematical terms, and by attempting to establish experimentally which interpretation of the formalism—if any—made more sense.

Today, wave-particle duality is part of the standard interpretation of quantum mechanics, and the "two-slit experiment" appears in most textbooks as the paradigmatic exemplar of the experimental consequences of this duality. As shown by Kristel Michielsen and Hans De Raedt in this volume, however, the two-slit experiment was formulated only much later as a thought experiment, and actually performed even later. If one looks at what was happening in the 1920s and '30s, the situation appears much less clear than what may seem today. For example, in 1928 Arthur Edward Ruark (1899–1979) proposed, "A critical experiment on the statistical interpretation of quantum mechanics" (Ruark 1928). Ruark's proposal was an experiment that at the time could not be performed, aimed at establishing whether a single atom could actually be in two states at the same time: if that was the case, claimed Ruark, then the atom might be able to emit light of two frequencies at the same time. This idea sounds quite strange today, but these reflections belonged to an earlier, fluid state of quantum mechanics in which the wave function was still regarded as a novel formal construct, which helped formulate predictions but was not necessarily physically significant in itself.

10 "ein atomares System [ist] stets nur in einem stationären Zustand [...] im allgemeinen werden wir in einem Augenblick nur wissen, daß [...] eine gewisse Wahrscheinlichkeit dafür besteht, daß das Atom im n-ten Zustand ist" (Born 1927, 171).

11 On the emergence of the statistical interpretation of quantum mechanics see Jammer (1966, 282–293).

Dirac's Symbolic Notation

After this short detour on experiment, let us go back to the way in which quantum theory developed in the late 1920s. Most theorists were not primarily interested in interpreting the formal apparatus of quantum mechanics, but rather in expanding it to fit a broader range of quantum phenomena. Many authors worked to this aim, and their results often merged with and built upon each other. I would like to conclude my short media archaeology of quantum theory by focusing on one author who was probably the most creative one in his manipulation of symbolic expressions: Paul Dirac (1902–1984). In my presentation I have suggested that different authors contributing to the emergence of quantum theory used different aesthetic strategies to develop and express their theoretical research. Many of Bohr's key research contributions were expressed in words and not in mathematical language, while other authors, as for example Schrödinger, employed traditional mathematical techniques, such as differential equations. More skilled mathematicians, like John von Neumann (1903–1957), used very refined mathematical structures as guidelines for their work on quantum theory, while Heisenberg, Born, and Jordan expressed their reflections in the form of innovative, and possibly nonrigorous, constructs: infinite matrices. Dirac's strategy in theoretical research was the manipulation of symbolic notation without much regard for mathematical rigor on the one side or physical sense on the other.[12]

Dirac's papers, especially those he wrote early in his career, are often a challenge to read. Unlike Heisenberg or Bohr, he offered hardly any verbal explanation of the reasoning behind his operations, and unlike Schrödinger or von Neumann, his manipulations of mathematical symbols cannot be understood in terms of any sharply defined mathematical structure. Yet Dirac reached his most significant results by taking symbolic expressions and transforming them to generate new physical-mathematical meanings (Borrelli 2010). On the basis of archival material Peter Galison has argued that much of what Dirac did with his formulas was guided by a visual and haptic intuition, which he did not express in his papers—a "secret geometry," as Galison wrote (Galison 2000). While this may be the case, it is also clear that Dirac paid great attention to the development of a symbolic notation that fittted his aims. It was not a notation linked to rigorously defined mathematical notions, but rather reflected the way in which he wished to manipulate the epistemic objects he was creating.

12 On Dirac's transformation theory see Jammer (1966, 293–307).

In 1927, while the new quantum theory was proving very successful in dealing with atomic and molecular systems and discussions about its statistical interpretation were underway, Dirac published a paper in which he proposed an extension of quantum mechanics to the treatment of phenomena that were not discrete, like atomic spectra, but rather continuous, such as collisions between particles. For handling discrete systems, matrices were appropriate representations, in that the rows and columns formally reflected the discontinuous nature of the states—but what about systems where energy and other quantities varied continuously? Dirac neither described physical considerations in words nor followed a rigorous mathematical path, but rather tackled the problem in terms of finding an appropriate extension of matrix notation.

His idea was in principle simple: in atomic theory rows and columns of matrices corresponded with discrete energy states, but in a more general theory they would have to relate to states of quantum systems having continuous values of energy or other physical quantities. Dirac did not ask what mathematical structure might correspond to a generalization of matrices, as Born and Wiener had done, but simply spoke of "matrices with continuous rows and columns" (Dirac 1927, 625) and wrote down symbolic expressions for them that were not backed up with any rigorous mathematical notion. Let us look in some more detail at one example of his work.

As we saw, quantum mechanics contained infinite matrices, and in the standard notation the symbol $g_{a,\,a'}$ represented the element of the matrix for quantity g whose rows and columns corresponded to the values of quantity a. Dirac now introduced the symbol $g_{a,\,a'}$, which visually conveyed the idea that it was the same as the matrix for g, but with continuous rows and columns. Matrices could be manipulated by sums of their elements, and Dirac manipulated "continuous" matrices in an analogous way using integrals. For example, the rule for multiplying two matrices g and f had the form:

$$(g \cdot f)_{\mathrm{a,b}} = \sum_{a'} g_{a,a'} f_{a',b}$$

In the case of "continuous" matrices, the rule for multiplying them became:

$$(g \cdot f)(\mathrm{a} \cdot b) = \int g(a,a')\, f(a',b)\, da'$$

When working with matrices, a necessary tool was the matrix usually represented by the symbol $\delta_{a,b}$, that is, a matrix having 1 on its diagonal and 0 at all other positions:

$$\begin{pmatrix} 1 & 0 & 0 & 0 & \ldots \\ 0 & 1 & 0 & 0 & \ldots \\ 0 & 0 & 1 & 0 & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \end{pmatrix}$$

This matrix was regarded as the "unity" matrix, since any matrix multiplied by it remained unchanged. What kind of expression could take up the same role for "continuous" matrices? It was here that Dirac introduced his perhaps most successful creation: the "delta function," often also referred to as Dirac's delta function. Dirac introduced the delta function in a paragraph bearing the title "Notation." I will quote the passage at some length: readers not familiar with the delta function need not try to understand what the characterization means exactly, but simply appreciate the tone of the text, which gives a very good idea of the nonchalant attitude Dirac had to mathematical rigor.

> One cannot go far in the development of the theory of matrices with continuous ranges of rows and columns without needing a notation for that function of a c-number *x* [NB c-number = complex number] that is equal to zero except when x is very small, and whose integral through a range that contains the point $x = 0$ is equal to unity. We shall use the symbol $\delta(x)$ to denote this function, i.e. $\delta(x)$ is defined by:
>
> $\delta(x) = 0$ when $x \neq 0$
>
> and
>
> $\int_{-\infty}^{+\infty} \delta(x) = 1.$
>
> Strictly speaking, of course, $\delta(x)$ is not a proper function of x but can be regarded only as a limit of a certain sequence of functions. All the same one can use $\delta(x)$ as though it were a proper function for practically all the purposes of quantum mechanics without getting incorrect results. One can also use the differential coefficients of $\delta(x)$, namely $\delta'(x)$, $\delta''(x)$..., which are even more discontinuous and less "proper" then $\delta(x)$ itself. (Dirac 1927, 625)[13]

Thus, Dirac thought of the introduction of the delta function as a question of notation: he clearly perceived his theoretical activity as the manipulation not of mathematical objects of physical quantities, but rather of symbolic

13 Readers familiar with the delta function will have noticed that what Dirac is defining here is actually what we today would refer to as $\delta'(x)$, but soon the labeling of the function was changed to the one usual today.

expression that carried a hybrid meaning. When the manipulation was completed, the results might be tested for mathematical soundness and empirical accuracy, and if the outcome was positive, all was well. This attitude can be found in many theoretical physicists, but Dirac brought it to a new level, and mathematicians heavily criticized the delta function especially until it was eventually given a rigorous definition.[14]

Axiomatic Definitions

One of the main critics of Dirac's delta function, and more in general of the flippant way in which the creators of quantum mechanics handled symbolic expressions, was von Neumann. In 1928 von Neumann published a seminal paper offering a rigorous, axiomatically defined version of quantum mechanics based on a notion he developed specifically for that purpose: abstract Hilbert spaces (von Neumann 1928).[15] At the beginning of that paper he criticized specifically the delta function, and wrote:

> [In the present quantum theory] one cannot avoid to allow also the so-called improper functions, such as the function δ(x) used for the first time by Dirac, which has the following (absurd) properties:
>
> $\delta(x) = 0$, for $x \neq 0$
>
> $\int_{-\infty}^{+\infty} \delta(x) = 1$[16]. (von Neumann 1928)

Other than Dirac, von Neumann saw the delta function—and also other symbolic expressions—as always carrying a mathematical meaning, and regarded it in this case as "absurd." Von Neumann was able to distill from the symbolic expressions involved in quantum mechanics some rigorous mathematical constructs, but ironically this success helped support the physicists' view that it was perfectly fine to play fast and loose with physical-mathematical expressions, as long as the final result was not incorrect: eventually, so physicists thought, some mathematician would come along and show that what physicists had done improperly could be done just as well in a proper mathematical way. Still today, even if a

14 The delta function is today rigorously defined as a distribution; see Jauch (1972).

15 For an overview on von Neumann's early work on quantum mechanics see Jammer (1966, 307–322).

16 Man kann nämlich nicht vermeiden, auch sogenannten uneigentliche Eigenfunktionen mit zuzulassen, wie z.B. die zuerst von Dirac benutzte Funktion δ(x), die die folgenden (absurden) Eigenschaften haben soll: $\delta(x) = 0$, für $x \neq 0$, $\int_{-\infty}^{+\infty} \delta(x) = 1$" (von Neumann 1928, 3). von Neumann's characterization of the delta function is the same as is usual today.

symbolic procedure appears questionable, its success is usually taken by physicists as an indication that it corresponds with a rigorous mathematical procedure that no one has yet had the time or inclination to discover (Borrelli 2012; 2015a; 2015b). This attitude has led to many significant physical results, but has also made the status of mathematical formulas as a privileged medium of theory increasingly stronger, as it helped disregard problems of rigor and coherence as temporary issues that would find a solution with time.

Epilogue: Bra and Kets

von Neumann's formulation of a rigorous, axiomatically defined mathematical apparatus for quantum mechanics was appreciated more by mathematicians then by physicists. Abstract Hilbert spaces eventually became the overarching formal constructs for defining quantum theory, but in physics research practice they were rarely utilized. The rather cumbersome formalism introduced by von Neumann in his papers found few, if any, followers, and his innovative mathematical ideas ironically ended up being usually expressed in terms of the "improper" notation Dirac had introduced in 1927 and later continued to develop further. It is worth taking a closer look at the evolution of this notation, as it provides further evidence of the importance of the aesthetic, in this case visual and haptic, dimension of (quantum) theory.

In his 1927 paper, Dirac had pursued his extension of matrix mechanics to "continuous matrices" by generalizing an idea that was at the core of Heisenberg, Born, and Jordan's theory: matrix transformation. The matrix associated with a given quantity g (e.g., position) with rows and columns corresponding to another given quantity a (e.g., energy) could be transformed into a matrix associated with the same quantity g, but whose rows and columns were associated with a quantity c, different from the original one. This was done by multiplying the original matrix by an appropriate "transformation matrix" T and its inverse T^{-1} according to the rule:

$$g_{c,c'} = \sum_{a,a'} T_{c,a}\, g_{a,a'}\, T^{-1}_{a'c'} \,.$$

For transforming matrices with continuous indices, Dirac simply wrote the symbolic analogous formula in which the sum was replaced by an integral, without worrying about what it might mean exactly in mathematical terms:

$$\mathrm{g}(a,a') = \int (a/c)\, \mathrm{g}(c,c')\, (c'/a)\, dc\, dc' \,.$$

This formula defined the symbol (a/c) as the continuous equivalent of the transformation matrix, a "transformation function," but left huge mathematical questions open. The matrix sum had already been problematic for infinite matrices, since it was unclear whether it would converge. Generalizing it to an integral without specifying what form the various terms included in it would have was even more problematic. However, the new notation had a very clear intuitive interpretation for readers used to working with infinite matrices. It is particularly interesting to note that the symbol (c/a) had no graphic equivalent in the formalism of the time. The symbol somehow visually and haptically suggested a matrix of which only the indices were visible—an object whose only aim was to substitute the indices a for c or vice versa.

One might be tempted to regard Dirac's procedure as an axiomatic definition of new physical-mathematical notions through the way they were manipulated, and in some sense that was what Dirac was doing. Yet he was doing it at the aesthetic level of symbolic notation, and not by employing the standardized logical-mathematical formalism of the time, as von Neumann would later do. One might claim a posteriori that abstract Hilbert spaces were already "implicit" in Dirac's symbols, but this would in my opinion misinterpret the historical constellation. At the same time it would also be incorrect to deny that von Neumann's axiomatic construction was largely building upon the constructs developed "improperly" in quantum mechanics.

In his textbook *Principles of Quantum Mechanics* ([1930] 1935) Dirac employed an only slightly modified version of the notation used in 1927 for transformation functions, but in 1939 he published a paper "On a new notation for quantum mechanics" in which he developed that symbolism further into the now ubiquitous "bra-ket" notation. In that paper Dirac explicitly stated the importance of notation (Dirac 1939), noting right at the beginning:

> In mathematical theories the question of notation, while not of primary importance, is yet worthy of careful consideration, since a good notation can be of great value in helping the development of a theory, by making it easy to write down those quantities or combinations of quantities that are important, and difficult or impossible to write down those that are unimportant. (Dirac 1939, 416)

The key idea of the bra-ket notation was to split the notation developed for the transformation function into two halves:

(a/b) → <a | b> which was the product of the bra <a| and the ket |b>.

As is clear both from their name and their graphic form, a “bra” and a “ket” were supposed to be combined with each other in a particular order, so that a haptic dimension joined the visual and auditory ones. Putting a ket in front of a bra was possible, but the resulting ket-bra would have very different properties from a bra-ket, as immediately conveyed by its peculiar appearance: |a> <b|. Readers familiar with the formalism of quantum mechanics will know that bras and kets today are regarded as representing elements of an abstract Hilbert space and of its dual, respectively, and there is no doubt that Dirac was exploiting those mathematical structures as a guideline, while at the same time avoiding any rigorous definition and leaving it to his new notations to promote useful, and to impede unimportant, terms.

Conclusions: Computer Simulations as a New Medium of Quantum Theory

I am now at the end of my overview of the many media that contributed to the construction of quantum theory: perspective drawings, simple arithmetic formulas, verbally stated physical principles, sets of numbers, the rows and columns of infinite matrices, differential equations, axiomatic logical-mathematical constructs and, last but not least, Dirac’s innovative symbolisms such as the bra-kets. Each author was free to choose the medium best suitable to his way of working and, especially in the early period, attitudes about what may or may not be acceptable as a “quantum theory” were very flexible—as long as correct results could be reproduced.

Can the employment of computer simulations to reproduce the results of quantum experiments without making use of the machinery of Schrödinger’s equation be seen as a practice belonging to the tradition of quantum theory I just sketched? It is my conviction that this is the case, and I hope that my presentation offered some material to broaden the discussion on that issue. I am convinced that computer simulations as a new medium of quantum theory might bring back some of the productive tensions present in early quantum physics.

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Discussion with Arianna Borrelli

Hans-Jörg Rheinberger: Thank you very much for your talk. The stage is open for questions, please.

Hans De Raedt: That was a very nice presentation by the way. So, I was always wondering, in a way quantum theory is nothing but linear algebra, and linear algebra was known since the time of Gauss. So why did it take so long for these physicists to realize that what they were doing was just a form of linear algebra?

Arianna Borrelli: Thank you. That is a very good question on the history of mathematics and physics. There are many historians of mathematics, including me, working on that topic. The answer to your question is that, in a sense, linear algebra has not been there since Gauss. If we think of linear algebra as abstract algebra, that is in terms of abstract Hilbert spaces and similar formally defined objects that were introduced by von Neumann... if we think of linear algebra in that sense, then there was no "linear algebra" before quantum theory. There were only what we see today as different implementations of abstract linear algebra, like in differential equations or matrix calculus.

Now, if historically at a certain time there is no formalized, abstract linear algebra, the historical actors clearly could not use it to connect all the different "implementations." Take the example of infinite matrices: we can think of them in terms of abstract algebraic structures, as "operators" in Hilbert space. But the historical actors saw them differently. John von Neumann, for example, or David Hilbert thought that if you have an infinite matrix which is bounded, then that is a mathematical object and you can do linear algebra with it. But if you have an infinite matrix which is not bounded, like those of quantum mechanics, a matrix about whose behavior you can say nothing, then that is not a mathematical object—I mean, it may be a mathematical object today for me or for you, but for the people at the time, such a matrix was not a mathematical object. And so one could not do any algebra with it.

In a way one may speak of a "thought collective" in Ludwik Fleck's sense (Fleck 1935). What seems obvious to us was not obvious to the "thought collective" of quantum physicists at the time.

HDR: Is it historically correct that Heisenberg, when he was writing down this so-called matrix algebra, was not aware of the fact that he was doing that?

AB: Yes, this is correct for the first paper, the one written by Heisenberg alone. The matrix formulation was brought in by Born and Pascual Jordan, who were familiar with the matrix formulas. However, Heisenberg was working with a formal analogy to Fourier series and the multiplication of Fourier series by convolution. That procedure has the same form as matrix multiplication. So it's again a question of how you want to look at it. Born and Jordan replaced the structure of Fourier series with matrices. That's a very interesting story and in a way it also shows how a formula is not just a formula: the same formula can have completely different meanings for different authors.

Martin Warnke: Thank you, this was really a very enlightening presentation about how contingent the ways are to grasp the phenomena by different formal methods. But what really struck me was that you reiterated the fact that the double-slit experiment was so late in conception and in practice. So this is really something that is not clear to me: Why this came so late? But the question now is: Have you any clue about the nature of this experiment? Since if, as we both do, we follow Dirac in saying that the apparatuses and experiments evoke what they measure, how could that be, that there is one experiment and one apparatus that evokes those complementary phenomena at the same time? Is it a sort of joined—linked—experiment and thought experiment around which everything we do, did yesterday, and are doing today is orbiting?

Have you got any clue about that?

AB: First of all I have to say when I was preparing this presentation I looked for some history of the double-slit experiment, but there is none yet—and I think someone should write it! What I can say now—and maybe those who have worked more with the experiment can say more about this—is that in this early period there was a lot of open discussion about how to… what term did you use? "Evoke", yes? So, the physicists had these equations and wanted to try to evoke something from them. The question is: What? What were they interested in "evoking" through the equations? We now think of particles or waves, but that was not the case then.

For example, Ruark, he saw these equations as a possible indication of the nonconservation of energy. Ruark thought of the Schrödinger equation as possibly saying that energy is only statistically conserved, that you could look and find evidence of energy nonconservation in single events—but that in the end it would average out. He was trying to think of a critical experiment showing whether there was or was not this nonconservation. That's what he was trying to "evoke," if you want: energy conservation or its opposite.

In the late 1920s people were trying to use thought experiments to better grasp what exactly the theory could or could not mean. And maybe the idea for the double-slit experiment could only come afterwards, when somehow the notion of particle-wave duality became more prominent. Only then one thought of an experiment evoking waves or particles.

Kristel Michielsen: I have one comment. There is a paper (Rosa 2012) that you could consider as an historical overview of these double-slit experiments. It appeared actually because of a discussion on whether a Japanese or an Italian group was the first to do the real electron double-slit experiment.

AB: Thank you!

KM: And then related to your question or comment, Martin, I would say in the two-slit experiment the wave and the particle do not appear at the same time. Because you see single events coming and then there's still no observation of wave character, and you have to wait for quite some time before you see the interference. So it's not at all a simultaneous appearance of waves and particles.

Lukas Mairhofer: I also rather have a comment, because I think that really with the diffraction from a crystal you could demonstrate that there is some wave nature of things that you always have been thinking of as particles. So maybe the double-slit experiment is not that big a step as you seem to describe it. Because there is also an interference phenomenon, the diffraction from a crystal, and putting in a double slit is just creating a different apparatus for doing interference experiments.

MW: But we are just talking about interferences, now. We are not talking about the other side, the particle. You are talking about the bra and not about the ket.

Eric Winsberg: Yeah, no I agree with you, I think the double-slit experiment is pedagogically beautiful in the sense that you don't really have to know very much about other physics to see both the particle and the wave existing in the same experiment. But yeah, there are experiments that are harder to understand, where you have to have more arguments that maybe, you know, a sophomore undergraduate can follow. But yeah, I think there really are experiments like that.

HDR: One more question: On your last slide you said that if you do computations we need the wave function collapse. I actually don't think that is true. You said "wave functions, wave collapse is still needed for the computation." Wave functions, certainly, but wave collapse, it is not needed: there is no computation where you actually use it—interpretation, yes.

AB: Well, I was referring to having first a formula with abstract Hilbert spaces and then at some point, when you have to do the measurement, you have to introduce the wave functions, and then the collapse, in that only one component wave function is left after the measurement, and that gives you the probability of the results. So you are right: one does not compute with the wave collapse, but assumes it to explain how you arrive at the prediction for the probabilities. So it is indeed interpretation.

Frank Pasemann: So perhaps just one comment on Dirac's delta: of course it is precise mathematics today, it is a simple example of distribution theory. Now because it's about history perhaps I can give a small story. It was on the occasion of Dirac's eightieth birthday, where almost every still living physicist of that time gathered together to celebrate his birthday at the International Centre for Theoretical Physics in Trieste, and there was a talk by van der Waerden, I think at that time a famous mathematician, on Schrödinger equation history. He mentioned a physicist in Dublin named Cornelius Lanczos, and he worked out that he had exactly the same equation and the difficulties with interpretation, and he was arguing that because he was not embedded in the famous German school with all the discussion on how to interpret it, he was not—you know—as famous as Schrödinger.

Now at the end of this talk I think Jürgen Ehlers, director of the Max Planck Institute of Physics in Munich at that time, stood up and said, "I'm happy to introduce Lanczos here, who is around." And so he was still living, was a very old man with very long white hair, and it was very funny, you know, that someone stood up and that's the guy who had a talk about himself and no one knew that he was still living. Okay.

Anne Dippel: I have one last question. You said at the end computer simulations are another medium and they could bring back the tensions, the creative tensions, into theory. How would you relate your statement to the talk we had yesterday by Hans De Raedt and Kristel Michielsen?

AB: Yes, I think computer simulations could play a similar role to Dirac's strange notation. It would be an example of a different strategy to represent or to make contact with the experimental results—a strategy that has already produced these tensions with respect to the usual representation in terms of Schrödinger equations. I think this was quite clear in the discussion yesterday. It was strange: the discussion took the form of classical physics against quantum mechanics, and the Bell inequality—and these are... I don't want to say old subjects, but these are discussions that have been spoken about a lot. I think that there is actually more. I believe that in what Hans and Kristel presented there is some new dimension from the point of view of a representation.

And this is to me similar to the strange notations of Dirac—of course in a completely different way, but from the epistemic point of view similar. Of Dirac's notation today we can say: "Oh, we have now shown that it was rigorous." But then, at the time, much of what Dirac was doing was not rigorous. And it was just different from the mainstream, it was the path that he had to take, in a sense, to try and expand the theory that was there. But this is just my take on it.

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