Data science of quantum phenomena and the development of quantum theory

Erik Deumens*

May 7, 2023

Abstract

Measurements of quantum phenomena provide data that have been organized and modeled using techniques of data science. The models used are rooted in the classical physics of Newtonian mechanics and Maxwell theory and use the concepts of particles and fields that are part of these theories of physics. They also use the notion of measurement used in classical physics. The data models are encoded into a set of postulates that are known as the Copenhagen formulation of quantum mechanics. The models are presented as the theory of quantum phenomena. Unfortunately, this formulation produces a number of paradoxes that have been the subject of debates for almost a century. The Einstein-Podolsky-Rosen paper, Bell's theorem, and the Kochen-Specker theorem and their experimental confirmation are two prominent examples of the paradoxical conclusions. Analysis shows that it is not surprising that data models lead to paradoxes. A deeper look at the physics taking place in a Stern-Gerlach experiment leads to an explanation of how the seemingly paradocical experimental results of violations of Bell and Kochen-Specker inequalities are produced by quantum dynamics.

This is note # 5 in a series of notes to untangle quantum mechanics for a general audience and experts alike.

URL https://people.clas.ufl.edu/deumens/files/pap-data-science.pdf

The textbooks of quantum mechanics present the student with a sequence of experiments that introduce quantum phenomena. The way the experiments are presented follows the historical formulation and highlighting the surprising character of the observations. This is natural and desirable because it makes the student go through the process of incorporating the new phenomena into the framework of everyday intuition. Classical theories are very much aligned with our intuition of the world. Newtonian mechanics is the prime

*Quantum Theory Project, University of Florida, ORCID 0000-0002-7398-3090

example as a theory of particles and macroscopic bodies, as well as continuous media with waves, such as sound waves in air and gravity waves in water.[1] Maxwell's electrodynamics is another example.

The methods of data science have become more widely known in recent decades. They show great power in organizing and working with data collected from a wide range of phenomena. It is useful to take a look at experiments on quantum phenomena as a data science activity.

All arguments in the debates focus on the results obtained from experiments on quantum systems; they are about data science. More precisely, they are about data science applied by people who work with the concepts of classical physics, formulated in terms of particles and waves. Crucially, the debaters also assume the validity of the concept of idealized measurement, but allowing for measurements to disturb the system.

Data science Let us look into that a bit deeper: It is the trail where no one researching the measurement problem has traveled before. In classical physics, the state of a system is described by sets of numbers: The position of a particle is a vector of three numbers, so is the momentum. The temperature of a system is a number, charge and mass are numbers. The state of a system, in Newtonian mechanics, at some time is described by a point in phase space, which is given as a list of the positions and momenta of all the constituent particles. A measurement by some device yields one of these numbers. Different devices can be constructed that have varying ability to get the number more of less accurately, but that is merely a technical problem, not a conceptual one for formulating the theory of Newtonian mechanics or for validating it by experiment.

Quantum experiments also give numbers, but there is an unavoidable probability associated with the observations. That, in and of itself is not a problem either, because probability methods have been used for centuries to determine the error of measurements. In classical mechanics it has always been assumed that the measurement error can be made as arbitrarily small. However, in quantum phenomena the error has a finite limit. This is most prominent for conjugate variables, like position and momentum, where the Heisenberg uncertainty relations express a fundamental limit [13].

The data science approach to understand where the observed correlations between measured values come from, how quantum systems "work," has led to attempts to build mechanical models in terms of these values. That approach has worked so well for all classical physics phenomena and has led to very successful theories. But it has not worked for quantum mechanics since no universal consensus about the theory has been reached.

Theory While the data scientists were figuring out how to make sense of the data and were modeling the apparently contradictory findings, Heisenberg [6] and Schrödinger [18] formulated the dynamical equation that captures the evolution underlying quantum phenomena, thus creating the new theory of quantum mechanics. Contrary to the "old

[1] Gravity waves should not be confused with gravitational waves in spacetime predicted by general relativity in 1915 and detected by LIGO in 2015.

quantum theory" of Bohr and Sommerfeld [19], this new equation gave correct results and has continue to do so for a hundred years. The equation is known as the Schrödinger equation, but the Heisenberg form of the equation is equivalent as was shown by Schrödinger [17]. The equation is formulated in terms of the "state" of the quantum system, which is defined as a vector in a Hilbert space; it is often represented in the form of function, called a "wavefunction." The Hilbert space is a mathematical construct, similar to the phase space that appears in the Hamiltonian formulation of Newtonian mechanics. One should focus there to build a theory for quantum phenomena. There one should look for an understanding of the various observed correlations in quantum phenomena, as was advocated in 1926 by the young Heisenberg. Considering the mathematics of matrix mechanics, Schrödinger's wave mechanics, and Dirac's transformation theory, the young Heisenberg said to Bohr "I just want to see where it leads." [11, p. 101]. His mentors, Bohr and Einstein, however, did not want to follow that approach. After 1926, in particular after formulating the uncertainty principle, Heisenberg fell in line with the general thinking about quantum mechanics and became an advocate of the Copenhagen formulation for the rest of his life.

The Copenhagen formulation states that the measurement process produces the values that are observed and that they are not possessed by the system independent of any measurement. It also denies the possibility of figuring out what happens with quantum systems during their evolution. Thus, it strictly adheres to the classical notion that the measurement process can be and should be viewed as outside of the dynamical evolution of physical systems. This is a highly suspect position to take in science, which claims to explore and explain *all* physical phenomena and processes. The constraint of keeping the epistemological status of experiment as ancillary leads to a particular approach for addressing the problem of whether systems have values independent being measured or not. Researchers looked for classical hidden variables that can take values but are not known, essentially extending the theory to include new variables.

Data theorems and experimental tests The debate about what this all means was highlighted in 1964 by Bell [2]. He opened the possibility to experimentally test whether the any of the models or theories using hidden variables could produce the observations of quantum phenomena. Such experiments were carried out by Clauser [9], Aspect [1], and Zeilinger [21]. They received the Nobel Prize in 2022 for that work. The experiments established that hidden variables can not provide the answer. However, the data-science mindset persists, and solutions are still being sought within the classical context of variables with values and a measurement process that can be effectively idealized as taking place outside of the dyanmics of the quantum world.

To strengthen the argument, Bell [3] and Kochen-Specker [14] formulated theorems on the data from observations of quantum phenomena. The theorems make no reference to any underlying physics concepts: no hidden variables, just data. These theorems are pure data science, as that term is used today. Budron *et al.* [7, p. 55] point out that the logic of such theorems, as part of data science before the term data science was used, was studied by Boole [4] already in 1862. As such the theorems are valid and general, but may not be as relevant to quantum mechanics as is generally accepted in the community of researchers interested in the foundations of quantum mechanics.

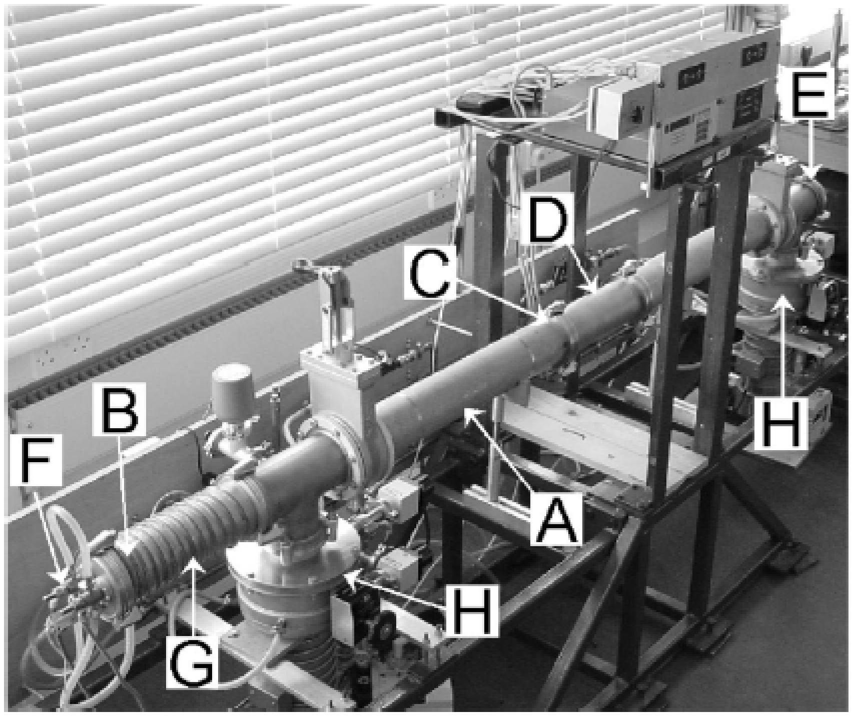

Figure 1: Photograph of the Stern–Gerlach experiment showing the flight tube A with the positions of the source B, collimating grid C, magnets D, and detecting slide E. Also indicated are the low tension connections F, cooling water channels around the source G, and the diffusion pumps H. (From Ref. [16])

Stern-Gerlach experiment We will now investigate in detail a very famous experiment that shows the peculiarities of quantum mechanics, namely the Stern-Gerlach experiment, first carried out in 1922 [10]. We will then perform the traditional modeling of the findings and then take a more in-depth look at the physics and, following Heisenberg's intuition, which is to follow the mathematical description given by the Schrödinger equation.

A modern version of the experiment that can be carried out in a student lab was designed by Porter, Pettifer, and Leadley [16]. We will consider that experiment to make the discussion concrete and specific. It will be clear that our conclusions apply to many quantum experiments. The physical setup is shown in Fig. 1. About 1 g of silver heated to a tenparature between 1200 K and 1500 K and the atoms effuse through some collimation towards a glass microscope slide 2 m away. The beam passes through a region with a magnetic field created by a set of 0 to 8 magnetic elements. The experiment is set up to produce eight beams at the same time. This has the advantage that one run explores different regions of field strength without the need for precise control of the beam, thus making the experiment simpler to build. Full details of the experiment can be found in Ref. [16]. After several days the silver deposits on the microscope slide look as shown in Fig 2.

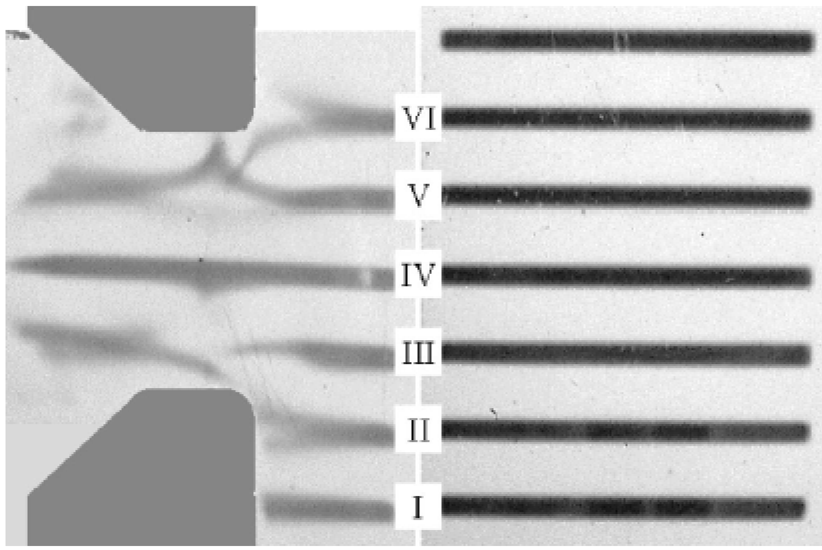

Figure 2: Pattern of deposited silver (dark areas) (right) without magnets and (left) with 6 magnetic elements and grid lines parallel to y-axis—the conventional Stern–Gerlach experiment. Separation of lines in the original image is 3 mm. (From Ref. [16])

Data-science viewpoint We will now describe the analysis of the observations from the Stern-Gerlach experiment that leads to the formulation of the Copenhagen formulation of quantum mechanics. We will see that it fits exactly what is now known as the data science approach. It should be noted that in the case of classical phenomena data science approach did lead to the known classical theories through intermediate stages like Kepler's Laws of Planetary Motion towards Newtonian mechanics.

The data scientist looks at the data in Fig 2(left) and sees the familiar splitting of the beam along the magnetic field for beams III and V. Other experiments have shown that the pattern is built up one atom at a time if the beam intensity is lowered sufficiently. In this experiment there are billions of atoms collected every second over the days of one run as the 1 g of silver is evaporated. The silver atoms come out of the evaporation chamber with a velocity around 650 m/s to 730 m/s, as determined from the Maxwell distribution of velocities[2] of atoms in a gas at temperatiures of 1200 K to 1500 K, respectively. A single atom of silver being deposited on the microscope slide is not detectable. Experiments that can detect individual events need beams with more energy.[3]

Hence the data scientist concludes that the silver atoms are particles flying through the region with the magnetic field and getting caught on the microscope slide. The atoms have their spin either up, i.e. aligned with the magnatic field, or down, i.e. aligned opposite. The atoms with spin up are deflected upward, the others wodward. In other words, the data scientist builds a model or theory from the observations that the atoms follow a definte trajectry from the oven where they are ejected through the magnetic field to the microscope slide where they are deposited.

But the Bell and Kochen-Specker theorems discussed above establish inequalities for measured results if indeed there is a definite spin for each silver atom from the moment it leaves the oven. The inequalities can be tested by experiments. Aspect, Clauser, and Zeilinger did carry out such experiments and these showed that quantum mechanics violates these inequalities. Therefore, the model proposed by the data scientist is wrong. The founders os quantum mechanics, as data scientists before the term was introduced, then invented the principle of particle-wave duality. That principle says that there is no classical trajectory but a fuzzy notion of something that acts like both at different times, depending on what experiment is being carried out. When results depend on the experiment, one what one is looking at, the results are called "contextual" by philosophers. This is how the Copenhagen formulation came to be. All interpretations of quantum mechanics are some distortion and elaboration of that formulation.[4]

The viewpoint Heisenberg did not pursue We will now pursue Heisenberg's intuition and "follow the math." In 1992, Daniel Platt presented a modern analysis of the Stern-Gerlach experiment [15]. He points out that many textbooks were still using the "old quantum theory" explanation of the experiment, i.e. the semi-classical Bohr-Sommrfeld quantum mechanics [19]. He provides an elegant description of what happens to a wavefunction when it moves through a magnetic field and shows that a single-bump wavefunction evolves into a shape with two humps, one with spin up and the other with spin down, moving toward the detector screen. This is the behavior familiar from the wavefunction evolving through a double slit and exhibiting multiple humps to make up interference fringes. Platt contrasts the description to the one in many textbooks using two classical paths, one with spin up and the the other with spin down.[5]

[2] The average velocity in the Maxwell distribution is given by $v = \sqrt{2kT/m} = \sqrt{2RT/M}$, where k is the Boltzmann constant, R is the gas constant, T is temperature in Kelvin, m is the particle mass, and M is the molar mass.

[3] A beautiful example experiment that shows individual events is the one by Tonomura *et al.* [20]; that experiment was analyzed in-depth, similar to the analysis in this note [8].

[4] The proponents of other interpretation will strongly disagree with that statement, but they have not been able to come up with anything better than the Copenhagen formulation to the extent that everybody can agrees with it.

[5] A good discussion on the measurement problem and the Stern-Gerlach experiment has been given by

With the understanding of how the Schródinger equation describes the evolution of the silver atoms from the oven to the microscope slide as the evolution of the wavefunction, we next focus on what happens when the atoms reach the glass slide. The assumption of the data scientist, and the founders of quantum mechanics, make the standard assumption in classical physics that the physical processes during a measurement can be safely idealized, and nothing of note happens. Following Heisenberg's intuition, we try to understand what the Schrödinger equation tells us about that. If that confirms the validity of the idealization assumption, that would be great progress. We will see that is shows that a lot more is going on than "just catching a silver atom."

To keep our analysis manageable, we will assume that the microscope slide is high quality glass: silica, i.e. pure SiO_2. The silver atoms have a velocity of about 650 m/s, which gives them a kinetic energy of 200 meV. When the silver atoms hit the silica glass slide, they stick by van der Waals forces to the slide surface, not by a chemical bond. That makes a structure that we denote by $Ag - (SiO_2)_N$ to indicate that the silver sticks to one or more silica molecules of the surface. The vand der Waals potentials for silica have a minimum around 126 meV to 600 meV depending on the angle from which the SiO_2 molecule is approached. Because the glass is at room temperature, the silica molecules also have an average kinetic energy of about 40 meV. With an average kinetic energy of 200 meV, the silver atoms will bounce off instead of sticking. We need a mechanism to distribute the energy from the silver to a number of silica molecules so that the silver atom gets decelerated and sticks. Maybe not all have to stick, but a good fraction must stick to make a visible record.

When the silver atoms evaporate from the silver beads, their wavefunctions are not precisely known. There is a probability distribution of wave functions. Because the wavefunctions are all generated the same way, they are all very similar. In other words, the statistical state of the beam of silver atoms has a small variance.

In contrast, the wavefunction of the microscope slide is not known precisely at all. This wavefunction describes the quantum state of a macroscopic number of silica molecules SiO_2 of the order of Avogadro's number 10^{23}. We have some macroscopic constraints on that wavefunction, such as the fact that the molecules are confined to the volume of the glass and that the glass in an amorphous solid state. Since the slide is at room temperature, the molecules are constantly moving, not moving far like in a liquid, but staying close to their site in the amorphous structure. The statistical state of the slide, therefore, has a probability distribution with a large variance in the space of slide wavefunctions.

The way the dynamics or mechanics of the process of detection is analyzed, i.e. the sticking of silver to the silica surface, proceeds by studying how any one wavefunction of a silver atom in the beam interacts with the wavefunction of the slide. If we look at this as an interaction between one silver atom and one silica molecule, we are running into the problem that the silver atom has too much energy and has little chance of being

---

Hannout *et al.* [12].

caught and sticking. The dynamics calls for a process where multiple silica molecules are involved that together can absorb the energy of the silver atom, leaving it with just the amount of energy to be at room temperature. Its kinetic energy, being proportional to the temperature, needs to drop from 200 meV to 40 meV in going from 1200 K to 300 K, respectively. The 160 meV that has to be taken from the silver atom has to be distributed over a sufficient number of silica molecules without heating them up significantly. For example, if we distribute it over four silica moelcules, each taking 40 meV, these four silica molecules would be at 600 K. They would then rapidly spread that energy to more silica molecules. This implies that the interaction that is described by the Shrödinger equation, as we "follow the math," is not between one silver and one silica molecule, or even four, but many more. If we assume that the temperature locally can rise by 3 K, a change of 1%, the kinetic energy involved is 0.4 meV. Then absorbing 160 meV in the dynamics that we need the Schrödinger equation to describe involves about $160/0.4 = 400$ silica molecules. Just looking at the nuclear degress of freedom involved, we count 3 for silver and $1200 = 3 \times 400$ for around 400 silica molecules. Thus, we expect that the dynamical process of detection of one silver by the microscope slide can be described by a wave function with about 1200 variables.

Because the wavefunction of the slide is giverned by a very broad probability distribution, the outcomes of the evolution computed by solving the Schrödinger equation with any pair of silver beam and silica slide wavefunction as initial condition will vary wildly. But when we take averages over the statistical state, i.e. over the probability distributions of the beam and the slide, we will find the obserbed results of silver atoms sticking to the microscope slide.

In principle, we have to solve the Schrödinger equation with all degress of freedom in the macroscopic slide with its 3×10^{23} degrees of freedom. However, our analysis shows that the dynamics happens in clusters with only about $N = 1200$ degrees of freedom. We can define a collective coodinate S, for "sticking," for that cluster that records the sticking of a silver atom. For example, it could be the distance from the silver atom to the closest point in the cluster of all $N = 1200$ silica molecules in the cluster. The coordinate is a function of all coordinates $S(X, Y, Z, x_1, y_1, z_1, \ldots, x_N, y_N, z_N)$. The value of $S = 0$, or similar, then indicates that the silver sticks. Because all coordinates are randomly distributed, the collective coordinate is also a random variable, but, by the famous theorem of large numbers in statistics and probablity, the variance of S goes like $\Delta S = 1/\sqrt{N} = 1/\sqrt{1200} = 3\%$. That means that the variable s has a narrow variance, even if the coordinates of the silver and silica atoms have typical quantum variances. In other words, the variable S behaves like a classical variable with a sharp value because the error is $\Delta S = 3\%$.

What we do not know yet is where the cluster is formed. The evolution of the statistical state driven by the Schrödinger equation using the full slide wavefunctions with all 3×10^{23} degrees of freedom does have that information. What we can say is that the probablity will be large that the clusters form at places where the wavefunction of the silver atom has a large amplitude, i.e. we discover Born's rule [5] from "following the math" as Heisenberg's intuition called for.

Conclusion Now we come to the true value of the 1926-notion of Heisenberg by giving insight beyond what the data-science approach has given. The reasoning above leads to a clear outcome from the evolution of the initial state of the spin-1/2 particle with the probabilities provided by the statistical state of the detector screen. There is no statistics in the wavefunction of the particle. It follows that for a physical system consisting of two correlated spin-1/2 particles the interaction with the statistical state of the screen will yield correlated results,[6] as experimentally observed. There is no need for any instantaneous collapse of the wavefunction.

With Heisenberg, following the mathematical framework for the physics behind quantum phenomena rather than following the approach of the data scientist, quantum mechanics becomes a full-featured theory of physics. The paradoxes turn out to be the result of forcing a classical model on the data obtained from observation of quantum phenomena.

References

[1] Aspect, A., Grangier, P., Roger, G.: Experimental Tests of Realistic Local Theories via Bell's theorem. Phys. Rev. Lett. **47**(7), 460–463 (1981). DOI 10.1103/PhysRevLett.47.460

[2] Bell, J.: On the Einstein-Podolsky-Rosen paradox. Physics **1**, 195–200 (1964)

[3] Bell, J.: On the problem of hidden variables in quantum mechanics. Rev. Mod. Phys. **38**, 447–452 (1966)

[4] Boole, G.: On the theory of probabilities. Phil. Trans. R. Soc. London **152**, 225–252 (1862)

[5] Born, M.: Zur Quantenmechanik der Stoßvorgänge. Zeitschrift für Physik **37**, 863–867 (1926)

[6] Born, M., Heisenberg, W., Jordan, P.: On Quantum Mechanics II. In: B.L. van der Waerden (ed.) Sources of Quantum Mecahnics, no. V in Classics of Science, pp. 95–137. Dover Publications, New York (1968). Original: Zeitschrift für Physik 35 (1926) 557-615

[7] Budroni, C., Cabello, A., Gühne, O., Kleinmann, M., Larsson, J.Å.: Kochen-specker contextuality. Rev. of Mod. Phys. **94**(4), 045,007 (62 pages) (2022)

[8] Deumens, E.: On Classical Systems and Measurement in Quantum Mechanics. Quantum Stud.: Math. Found. p. 37 pages (2019). DOI 10.1007/s40509-019-00189-3

[6] The mathematical details are described in reference [8].

[9] Freedman, S., Clauser, J.: Experimental test of local hidden-variable theories. Phys. Rev. Lett. **28**, 938–951 (1972). DOI 10.1103/PhysRevLett.28.938

[10] Gerlach, W., Stern, O.: Der experimentelle Nachweis der Richtungsquantelung im Magnetfeld. Zeit. Phys. **9**, 349–352 (1922). DOI 10.1007/BF01326983

[11] Gilder, L.: The Age of Entanglement when Quantum Physics was Reborn. Vintage Books, New York (2008)

[12] Hannout, M., Hoyt, S., Ktyowonos, A., Widom, A.: Quantum measurement theory and the Stern-Gerlach experiment. Am. J. Phys. **55**(5), 377–379 (1998). DOI 10.1119/1.18876

[13] Heisenberg, W.: Über den anshaulichen Inhalt der quantentheoretischen Kinematik und Mechanik. Zeitschrift für Phsyik **43**(3), 172–198 (1927). DOI 10.1007/BF01397280

[14] Kochen, S., Specker, E.P.: Theproblem of hidden variables in quantum mechanics. J. Math. and Mech. **17**, 59–87 (1967). DOI 10.1512/iumj.1968.17.17004

[15] Platt, D.E.: A modern analysis of the Stern-Gerlach experiment. Am. J. Phys. **60**(4), 306–308 (1992). DOI 10.1119/1.17136

[16] Porter, J., Pettifer, R.F., Leadley, D.R.: Direct measurement of the transverse Stern-Gerlach effect. Am. J. Phys. **71**(11), 1103–1108 (2003). DOI 10.1119/1.1574321

[17] Schrödinger, E.: Über das Verhältnis der Heisenberg-Born-Jordanschen Quantenmechanik zu der meinem — On the relation between the quantum mechanics of Heisenberg, Born, and Jordan and that of Schrödinger. Annalen der Physik **384**, 734–756 (1926). DOI 10.1002/andp.19263840804. Original in volume 79

[18] Schrödinger, E.: Quantisation as a Problem of Proper Values (Part I). In: E. Schrödinger (ed.) Collected papers on Wave Mechanics, pp. 1–12. Chelsea Publishing Company (1982). Original: Annalen der Physik 79 (1926) 489-527

[19] Sommerfeld, A.: Atombau und Spektrallinien. Friedrich Vieweg und Sohn, Braunschweig (1921). First edition 1919. Reproduced by Nabu Public Domain Reprints

[20] Tonomura, A., Endo, J., Matsuda, T., Kawasaki, T., Exawa, H.: Demonstration of single-electron buildup of an interference pattern. Am. J. Phys **57**(2), 117–120 (1989)

[21] Weihs, G., Jennewein, T., Chistoph, S., Weinfurter, H., Zeilinger, A.: Violation of bell's inequality under strict einstein locality conditions. Phys. Rev. Lett. **81**(23), 5039–5043 (1998). DOI 10.1103/PhysRevLett.81.5039