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About Waves, Particles, Events, Computer Simulation, and Ethics in Quantum Physics

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When Max Planck in 1874 asked one of his teachers, Philipp von Jolly, whether to choose physics as his discipline of academic study, he received the response that there was not much to be gained there. This trivia about Planck's life and the course of the history of science he himself influenced so much tells us: we never should be too sure that the gaining of knowledge is ever finished.

Despite von Jolly's opinion the beginning of the twentieth century brought about several surprises: with the appearance of Herman Minkowski's concept of space-time and Albert Einstein's annihilation of the ether that in the end led to the special and later the general theories of relativity, a first radical new branch of physics appeared. It was counterintuitive and yet scientifically highly successful at the same time. It revealed insights to the concepts of space and time and to problems of cosmology, to the very big of what we call "nature". But the high hopes that humankind would also soon know how to get hold of the world of very small were disappointed initially. The radiation of atoms and the behavior of subatomic particles that were discovered by that time seemed so strange that it was utterly unexplainable by contemporary physics of that period of time.

Then, as a second scientific surprise to the young century, that was about to shock humanity with an abundance of violent events in its further course, quantum mechanics entered the realm of physics.

Quantum mechanics, originally a theory developed by Planck to describe the black-body radiation problem, soon helped to explain atomic and subatomic phenomena. It had been evolving alongside experimental setups to a point of completion at the beginning of the 1930s. Thus, it provided new possibilities in describing the material world with a precision that was not achievable before. Nevertheless, it encoded into physics a rich collection of riddles and paradoxes, like the simultaneity of wave and particle perspectives, of "spooky actions at a distance," known as quantum entanglement, the decline of determinism, and the impossibility of simultaneously and exactly measuring well-known quantities like the location and velocity of a particle.

Physicists like Einstein were not satisfied with this situation of logical and conceptual inconsistencies—he once wrote "God doesn't play dice with the world"—and throughout the 20th century for beginners and lay people, as well as for experts such as the famous inventor of the diagrams for the interaction of subatomic particles named after him, Richard Feynman, the bewilderments of quantum theory are hard to accept on the one side and an invitation to esoteric speculation on the other. How can a thing be at the same time a wave and a particle? How can the state of one thing influence another instantaneously even though they are in two different, distant places? On the other hand, today, quantum mechanics proves to be the best tested theory in the history of physics. Therefore, experimentalists and theoreticians simply get used to the formalism that yields excellent predictions through the course of their education, and have to suppress the logical problems, since it works in the lab, and the lab has to work. The presuppositions about the behavior of nature turn into facts.

In the quantum world particles interact at a distance, and numerous experiments show, that they act as if under a spell of contagion cast by a witch. But science is not magic, and how can we understand nature to the fullest, when we're part of the system? The subatomic world seems to be formally describable, but from a logic perspective ungraspable for modern human beings. Even more when they are relying on logical devices such as the computer itself.

Physics students learn to deal with the ungraspable aspects of their discipline; many succumb at one point or another to the slogan "Shut up and calculate!" to cope pragmatically with the open problems of quantum mechanics, and even more so as their military and industrial applications require ever more young people being trained in it. Others try to overcome the theoretical problems by building experiments. This seems to suggest that pondering the philosophical implications and logical problems of quantum mechanics might be superfluous, since the math works and the experiments are producing results. The common attitude towards a mathematical apparatus that works so well reminds us of Martin Heidegger's prejudice about the sciences as disciplines that seem not be able to "think", because they "do", we might add.

Since the beginnings of quantum theory, thought experiments especially served as tools to work out the contradictions and peculiarities between a reasonable Newtonian world in which humans would live, and a theory of microscopic cabinet of wonder where nature shows its magic side. Of these experiments the one about the double slit is the most famous, the simplest and the one in which experimentation, theory, and computer simulations still meet with vivid intensity. It observes how particles behave if shot onto a twofold opening that allows for alternatives in their trajectory. Surprisingly enough, single particles produce interference patterns that are known, since then, to be phenomena of waves alone.

This experiment is usually attributed to the fundamental idea that individual elementary particles behave like waves, because the interference patterns on a screen far from the double slit only emerge if we do not know which of the slits they passed through, one by one. Since the introduction of the de Broglie wavelength and Schrödinger's matter wave equation, there is even the strong suggestion that seemingly indivisible particles pass through both slits at the same time.

The logical difficulty arises when an interpretation of the double-slit experiment tries to theorize individual particles that behave on their way through the experiment as if they were smeared out in space, although they are detected at distinctive places in the end. The concept of a matterwave and its inherent idea of self-interference of particles is hard to reconcile with measurements that in the end take place event by event. The notion of the event itself does not appear in traditional quantum theory, and at the end and the beginning of the experiment, in its Newtonian moment, matter shows itself as solid, not wavy, while in-between, the jiggly aspect of matter itself seems to appear; without that it can't be theorized.

Although the predictions of quantum theory show excellent experimental confirmation, quantum theory is not capable of describing the measurement process itself on the mathematical level. It is said that the wave function "collapses" at the event of the measurement, indicating the end of the quantum formalism. In the lab this normally takes place through the experimental observation of individual events, for example, the click of a detector. Quantum theory only allows for statistical predictions that can be tested by large numbers of measurements, never to statements about single events.

Now enter computer simulations!

With the development of event-based computer simulations new opportunities arise to describe the behavior of singular molecules as observed in quantum optical experiments of the double slit type. At the Institute for Advanced Study on the Media Cultures of Computer Simulation (MECS) in Lüneburg, Germany, we held a conference on the 20th and 21st of January 2016 to explore the contradictory phenomena of interferences and events from a logical perspective, as well as the dichotomy of the wave and particle images that quantum physics demands we deal with. We invited distinguished scientists and scholars from the fields of computational, theoretical, and experimental physics, and of the history and philosophy of science, in order to explore the potential of concepts and technologies emerging out of computer simulations to tackle unsolved problems at the theoretical heart of contemporary quantum mechanics. Can simulations not only provide descriptions and predictions for physics behavior, but also produce theories in their own right, which could compete with traditional theoretical concepts such as a differential equation-based theory of quantum mechanics?

In the interdisciplinary audience there were physicists, computer scientists, philosophers, game theorists, and scholars of literature, who would critically examine the presentations and contribute to the intense discussions that brought fresh perspectives on the epistemological role of computer simulations in physics and science in general, but also showed the robustness of contemporary quantum mechanical experimentation and theory.

By metaphorically using a quantum physics notation in the title of the conference, the <bras| and the |kets> of Paul Dirac, we illustrated our attempt to find out how much interference could be found in its opposing notion of events— and vice versa— by projecting them onto one another as: <interferences|events>, pronounced as "bra interferences ket events." In quantum mechanics such a term computes to what extent the state on the right, the |ket>, could be projected onto the state on the left, the <bra|. Arianna Borrelli wrote about this in her paper in this book. If there is a nonzero result for this quantum mechanical term—to use the slang of the discipline—then we would know more about the relationship between

those contradictory concepts and could then calculate the probability that one turned into the other.

Indeed, we found much more than just the void! This book documents the enlightening presentations and intense discussions we had during those two days. The table of contents follows the conference proceedings by thoroughly picturing the concurrent streams of thought that the subject ignites in people's minds. All the material and arguments are comprehensible to a wider audience and provide explanations that do not need a scientific education as a prerequisite. Formulas only appear as subjects of methodological investigation, and the arguments are made plausible without using the language of math.

Our first speakers, Kristel Michielsen and Hans De Raedt, both theoretical and computational physicists at the Jülich Research Centre talked about their approach to theory building and description of the aforementioned double-slit thought experiment—also actually performed in a lab later on—through the use of event-based computer simulations. Differently from the traditional approach of quantum mechanics, they model the whole process using events. A messenger is emitted by a source and processed by the experimental apparatus in a way that can be described by simple rules. At the end a sequence of individual events triggers a detection device that stands in for the measuring detectors in a laboratory. Instead of using the matrix- or differential equation-based mathematics developed by Werner Heisenberg, Erwin Schrödinger, Dirac and others that does not explain the behavior of single events but of collectives alone, a computer piles up results of discrete processes modeled by algorithms that then look similar to, if not indistinguishable from, laboratory data. In Michielsen and De Raedt's approach, everything is deterministic and there are no logical oddities in the whole process, unlike with the formalism of quantum physics that is normally applied without exception throughout the discipline. At the same time the results of the experimental quantum mechanical setups are perfectly reproduced. The tradition of logical reasoning based on computer simulations is put to an extreme perfection, ruling out all "spookiness" of quantum mechanics through media technology.

This marks the fascinating aspect of an event-based simulation attempt like the one described here: it only considers undoubtable properties of particles like their mass or spin, makes reasonable assumptions about experimental devices and does not rely on the so-called first principles used everywhere else, like the uncertainty principle or quantum states that can exist in superpositions as solutions to the Schrödinger equation in quantum theory. These principles are known as such because they are claimed to be the all-encompassing laws of a field that always hold true and from which all phenomena can be deduced. First principles have a similar grounding role as axioms in mathematics, but still have to stand an experimental test. The event-by-event approach is unparalleled in the hundred years of quantum research up to now, and only became possible because of the computing solutions available since the last three decades. This also means that physicists do not know through experience how far they can trust this method in cases where they do not have data from the lab. The only strategy to confirm the approach is to play a Turing's imitation game on the microscopic level, to judge just by the data what is a simulation and what is a lab process. If one cannot tell them apart, one may have to concede some credibility to this novel approach and place it as a computational solution alongside the existing mathematical approaches to describe the phenomena traditionally called "quantum."

At stake is the epistemological question of what relation exists between any formalism, be it traditional mathematics or novel computer simulations, and "nature" itself. Or, how cultural are the physical approaches to defining nature? Do mathematical theories of any kind say anything about nature itself or are they conceptual metaphors we learned to "live by" (Lakoff and Johnson [1980] 2003)?

The discussion after the presentation raised questions on the inclusion of the measurement event into quantum mechanics that in its current condition cannot deal with events at all, e. g. could not include the measurement operation itself. Subsequently was a debate about the collapse of the wave function, indicating the very border of the quantum formalism. Is there a "classical" world where the event of a measurement takes place and a separate "quantum" world where we have interferences from individual particles? The views on that differed across the audience.

Lukas Mairhofer, currently based in the Lukas Arndt-Group at Vienna Center for Quantum Science and Technology of Vienna University, gave the next presentation, on observing the unobservable and the quantum interference of complex macromolecules. Not only does Mairhofer reflect his work as a philosopher, he also does so as a passionate experimentalist. He provides a reflected glimpse into the contemporary practices of quantum mechanics, using multiple-slit experiments in the lab, where theoretical perspectives guide experimental work at any time. In a quantum mechanical experiment the logical problems of quantum theory turn into those of "practical" labor: the physicists fill one side of a complex technical apparatus with a grainy material consisting of visible particles—and nevertheless are forced to assume that it behaves like a matter wave on the way through the experimental system, passing optical grids where every molecule interferes with itself. At the end the detector counts discrete clicks that sum up to an interference patterns of a wave phenomenon. Contrary to the event-by-event simulative approach of the speakers before is the use of traditional quantum mechanics as the grounding theory. But Mairhofer and the whole Vienna Quantum Optics group go well beyond what could be done theoretically nowadays: they measure in regions where theoretical calculation is still impossible. Experimental verification is at the very core of the epistemic process in physics, and so the quantum optical setups in Vienna provide crucial indications of what could be known in the science of physics.

In the discussion experimental details were explored and philosophical questions were debated, such as the translation of subatomic behavior into the "classical world": What would it mean to be delocalized as a human being, as during the quantum mysteries of matter spread out in space as a matter wave? Mairhofer ends his talk with a prospect: What would it mean if living matter, like viruses, was subject to self-interference in the double-slit experiment?

Since in a contemporary quantum optical laboratory an experimental setup without computers is impossible, theoretical questions about media arose: What is the contribution of contemporary simulations to quantum optical experiments? Is what Mairhofer does in his experiments in itself already a simulation? What relationship exists between experiment and computer simulation in general? Is experimentation more of a simulation than science believed it to be up to now?

The next speaker, Mira Maiwöger, works as an experimental physicist in the Atomchip group of Jörg Schmiedmayer at the Atominstitut in Vienna. In her experiments the concept of matter waves also takes an important role. Her experiment investigates so-called Bose–Einstein condensates (BECs), which come into being, according to quantum theory, when big lumps of matter, say a spoonful, assemble in one big quantum state. This happens when matter is cooled down to extremely low temperatures. The speciality of her experiment is to prepare matter under extreme conditions, creating states that are also interesting theoretically, and then drawing conclusions for other materials that cannot be forced into these modes of existence in the same way. Experimentation becomes a kind of simulation of one system by another.

Maiwöger explains how one simulates magnetic material by observing BECs in rubidium. This analog simulation does not use algorithms to mimic a system of interest, but exploits the concept of similitude, of vicarious relationships.

Since all that work is embedded into a theoretical context, one which claims that particular systems are similar in a conceptual respect, the experiments not only probe physical systems but also physical theory, all this by analog simulation. To take one example, there is the theoretical concept of the superposition of states, say a right turning and a left turning one, essential to quantum mechanics and yet absolutely impossible from the perspective of classical physics, where something cannot turn right and left at the same time. To directly deal with these phenomena is like bringing the disturbing aspects of quantum physics into a material, directly observable being, all without taking resort to computers.

In the vivid discussion on the work currently done at the Viennese Atominstitut, philosophical aspects of the onto-epistemology of the quantum world explored by Karen Barad were elucidated. The framework of "agential realism" (Barad 2007) delivers a fruitful approach to also understanding why event-based simulations could equally explain the seemingly contradictory subatomic world of the from a classical perspective. Maiwöger showed what "non-natural nature," or natureculture (Law 2010), itself could actually be if put under the conditions of experimental physics: obviously it is not the privilege of computer simulations to create artificial realities, but as has been stated throughout the last decade by researchers from different fields in the realm of science and technology studies, physics itself produces realities that are neither pure nature, nor culture.

One goal of the conference was to clarify the relationship between event-based computer simulations and physical theory. As trained theoretical physicist and expert in building, as well as simulating robots with computers, Frank Pasemann from Osnabrück University seemed to be the right person to ponder about a possible need for new kinds of theory with the presence of computer simulations in theoretical physics. He showed some criteria of sound physical theories to discuss whether computer simulations themselves could be thought of as theories on their own, but remains undecided on the matter and expects further evidence in the future. Nevertheless, he states the obvious influences of computer simulations on theory building in physics, the full consequences of which are not yet known.

In the discussion afterwards comparisons with other disciplines such as biology helped to question whether researchers are used to describing phenomena without having something that could be called a theory altogether, and how theoretical trends and habits emerge and vanish over time.

The next speaker, Arianna Borrelli, a historian of physics and a trained physicist herself, working at the MECS as well as at the Technical University of Berlin, gave us impressions from the history of quantum physics about how contemporary computer simulations might be regarded as a type of theory. She did that by pointing us to the creative functions of notation; how the notions of a theoretical framework are actually written down normally slips our attention. She described the eminent role that a specific form of the expression of abstract concepts plays in the development of a physical theory, for example, notational systems as media that influence our thinking. Interestingly enough even the concrete forms of such expressions seem to have haptical and sensual sides to them and can be regarded as "embodied theories." She showed this by recalling that the algebraic terms for the atomic spectra of radiation entered science unexpectedly by the way of perspective drawings, and that Dirac and others bent mathematical concepts far beyond the areas justified by mathematical proof in order to invent physically "interesting" notations, done so by using infinite or even continuous matrices.

From that perspective, computer simulations could be seen as another way of embodying theoretical concepts into a different material form, equally as valid as mathematical notations.

In the following discussion the close resemblance between creative notational methodologies and computer simulations became much clearer. The stage was now set for an even broader perspective on the vicarious relationships between different areas of scientific research. Having started <interferences|events> with the question about in which way event-based computer simulations could be producing physical theories in their own right, the conference now realized that this was not the only structure for exploiting the similitude between different parts of physical science. Not only computer simulations stand in for physical systems: One physical system mimics another, notational formalisms are precursors to mathematics, and, as we will see, one theory can stand in for another.

Leuphana-based media theorist Wolfgang Hagen gave a historiographical account of how Heinrich Hertz was simulating electromagnetism using elasticity theory. He explored the transitions between those fields and showed a historical example of a very conscious and skeptical use of parallelisms between fields of knowledge. The similitude and the analogy didn't need to be perfect in every aspect; the incompleteness of any formalism describing nature was much clearer in Hertz's times than it is nowadays, when theory becomes so successful that it seems to be without alternative.

Again Barad's concept of agential realism served as a discursive springboard to discussing the ethics of "not knowing" and the impact of media on scientific interventions and representations, as well as the relationship between nature and culture. Finally, the discussion turned again to the central topic pursued at MECS, which is the influence of computer simulations on scientific thinking, of how to think of them as "inneres Scheinbild" (mental images) in the way Hertz used the term.

The last presentation of the conference was an intervention by historian of science and biologist Hans-Jörg Rheinberger, who emphasized the special epistemological status and role of experimental systems. He asked stimulating questions, such as: Would it be possible for computer simulations to produce new knowledge about nature as explorative experiments do? What is the relation between computer simulations and thought experiments? And if, like Niels Bohr put it, theory is on what we know about nature and not about nature itself, what then are computer simulations? Finally, could quantum theory be seen as an experimental way of knowing?

The general discussion led us back to the work of Michielsen and De Raedt, reiterating the questions about ontology and the realm of theoretical description overall.

This last roundtable served to sum up the thoughts of the participants. Computer simulations as creators of a new type of theory could open up the discovery of new phenomena unseen by traditional theories and should be included by the experimentalists in their research. A glimpse into the history of science and of disciplines other than physics, such as biology, shows that different relations between theory and experimentation or discovery in general evolve during the course of the history of an academic discipline. A great deal of complexity and richness is lost if the only guide to discovery is what traditional theory is pointing us to and what published scientific papers reveal from the research process. Also inspired by biology the question arose of what life is if it gets into the computer? How does mathematics relate to the state of being alive?

The discussion touched on the plurality of today's approaches in physics and how by mutual inspiration different fields such as computational and quantum physics could end up finding new insights by testing computational-based hypotheses on the one hand and analyzing experimental data thrown away before—because they were thought of as "useless", that is, not complying to traditional theories—on the other.

The crucial loop between theory and experiment, the quest for reproducibility, the whole epistemological apparatus of a positive, exact science, now seemingly enter into a crisis because of experiments that are very difficult or even impossible to reproduce.

At the end of the conference the importance of ethics with regard to the impact of computer simulations in science brought together all the disciplines assembled here, asking for an interdisciplinary approach that would lead to the establishment of ethics of design in simulation—thoughts that are related to discussions already led by Bertolt Brecht and Hans Reichenbach in the early era of quantum mechanics.

The times when it was enough to "shut up and calculate" are over. While computer-simulations contributed to the climate of "philosophobia" in physics in the first place, new modes of doing simulations are opening long-time black-boxed topics of how this discipline conceptualizes nature and the relation of the observer to what can be observed. Go ahead and start to think anew by reading yourself what the participants of <interferences|events> had to say.

References

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