Machines Learn Chemistry

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A new tool is drastically changing the face of chemical research – artificial intelligence. In a new paper published in Nature, researchers review the rapid progress in machine learning for the chemical sciences. [25]

A new type of artificial-intelligence-driven chemistry could revolutionise the way molecules are discovered, scientists claim. [24]

Tired of writing your own boring code for new software? Finally, there's an AI that can do it for you. [23]

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Understanding how a robot will react under different conditions is essential to guaranteeing its safe operation. [21]

Marculescu, along with ECE Ph.D. student Chieh Lo, has developed a machine learning algorithm—called MPLasso—that uses data to infer associations and interactions between microbes in the GI microbiome. [20]

A team of researchers from the University of Muenster in Germany has now demonstrated that this combination is extremely well suited to planning chemical syntheses—so-called retrosyntheses—with unprecedented efficiency. [19]

Two physicists at ETH Zurich and the Hebrew University of Jerusalem have developed a novel machine-learning algorithm that analyses large data sets describing a physical system and extract from them the essential information needed to understand the underlying physics. [18]

Now researchers at the Department of Energy's Lawrence Berkeley National Laboratory (Berkeley Lab) and UC Berkeley have come up with a novel machine learning method that enables scientists to derive insights from systems of previously intractable complexity in record time. [17]

Quantum computers can be made to utilize effects such as quantum coherence and entanglement to accelerate machine learning. [16]

Neural networks learn how to carry out certain tasks by analyzing large amounts of data displayed to them. [15]

Who is the better experimentalist, a human or a robot? When it comes to exploring synthetic and crystallization conditions for inorganic gigantic molecules, actively learning machines are clearly ahead, as demonstrated by British Scientists in an experiment with polyoxometalates published in the journal Angewandte Chemie. [14]

Machine learning algorithms are designed to improve as they encounter more data, making them a versatile technology for understanding large sets of photos such as those accessible from Google Images. Elizabeth Holm, professor of materials science and engineering at Carnegie Mellon University, is leveraging this technology to better understand the enormous number of research images accumulated in the field of materials science. [13]

With the help of artificial intelligence, chemists from the University of Basel in Switzerland have computed the characteristics of about two million crystals made up of four chemical elements. The researchers were able to identify 90 previously unknown thermodynamically stable crystals that can be regarded as new materials. [12]

The artificial intelligence system's ability to set itself up quickly every morning and compensate for any overnight fluctuations would make this fragile technology much more useful for field measurements, said co-lead researcher Dr Michael Hush from UNSW ADFA. [11]

Quantum physicist Mario Krenn and his colleagues in the group of Anton Zeilinger from the Faculty of Physics at the University of Vienna and the Austrian Academy of Sciences have developed an algorithm which designs new useful quantum experiments. As the computer does not rely on human intuition, it finds novel unfamiliar solutions. [10]

Researchers at the University of Chicago's Institute for Molecular Engineering and the University of Konstanz have demonstrated the ability to generate a quantum logic operation, or rotation of the qubit, that - surprisingly—is intrinsically resilient to noise as well as to variations in the strength or duration of the control. Their achievement is based on a geometric concept known as the Berry phase and is implemented through entirely optical means within a single electronic spin in diamond. [9]

New research demonstrates that particles at the quantum level can in fact be seen as behaving something like billiard balls rolling along a table, and not merely as the probabilistic smears that the standard interpretation of quantum mechanics suggests. But there's a catch - the tracks the particles follow do not always behave as one would expect from "realistic" trajectories, but often in a fashion that has been termed "surrealistic." [8]

Quantum entanglement—which occurs when two or more particles are correlated in such a way that they can influence each other even across large distances—is not an all-or-nothing phenomenon, but occurs in various degrees. The more a quantum state is entangled with its partner, the better the states will perform in quantum information

applications. Unfortunately, quantifying entanglement is a difficult process involving complex optimization problems that give even physicists headaches. [7]

A trio of physicists in Europe has come up with an idea that they believe would allow a person to actually witness entanglement. Valentina Caprara Vivoli, with the University of Geneva, Pavel Sekatski, with the University of Innsbruck and Nicolas Sangouard, with the University of Basel, have together written a paper describing a scenario where a human subject would be able to witness an instance of entanglement—they have uploaded it to the arXiv server for review by others. [6]

The accelerating electrons explain not only the Maxwell Equations and the Special Relativity, but the Heisenberg Uncertainty Relation, the Wave-Particle Duality and the electron's spin also, building the Bridge between the Classical and Quantum Theories.

The Planck Distribution Law of the electromagnetic oscillators explains the electron/proton mass rate and the Weak and Strong Interactions by the diffraction patterns. The Weak Interaction changes the diffraction patterns by moving the electric charge from one side to the other side of the diffraction pattern, which violates the CP and Time reversal symmetry.

The diffraction patterns and the locality of the self-maintaining electromagnetic potential explains also the Quantum Entanglement, giving it as a natural part of the relativistic quantum theory.

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Author: George Rajna

Preface

Physicists are continually looking for ways to unify the theory of relativity, which describes largescale phenomena, with quantum theory, which describes small-scale phenomena. In a new proposed experiment in this area, two toaster-sized "nanosatellites" carrying entangled condensates orbit around the Earth, until one of them moves to a different orbit with different gravitational field strength. As a result of the change in gravity, the entanglement between the condensates is predicted to degrade by up to 20%. Experimentally testing the proposal may be possible in the near future. [5]

Quantum entanglement is a physical phenomenon that occurs when pairs or groups of particles are generated or interact in ways such that the quantum state of each particle cannot be described independently – instead, a quantum state may be given for the system as a whole. [4]

I think that we have a simple bridge between the classical and quantum mechanics by understanding the Heisenberg Uncertainty Relations. It makes clear that the particles are not point like but have a dx and dp uncertainty.

Predicting reaction results: Machines learn chemistry

Everyday life without artificial intelligence is barely conceivable in today's world. Countless applications in areas such as autonomous driving, foreign language translation or medical diagnostics have found their way into our lives. In chemical research, too, great efforts are being made to apply artificial intelligence (AI), also known as machine learning, effectively. These technologies have already been used to predict the properties of individual molecules, making it easier for researchers to select the compound to be produced.

This production, known as synthesis, usually involves considerable effort as there are many possible synthesis routes to producing a target molecule. Since the success of each individual reaction depends on numerous parameters, it is not always possible, even for experienced chemists, to predict whether a reaction will take place—and even less how well it will work. In order to remedy this situation, a team of chemists and computer scientists from the University of Münster (Germany) has joined forces and developed an AI tool which has now been published in the journal *Chem*.

Background and method:

"A chemical reaction is a highly complex system," explains Frederik Sandfort, Ph.D. student at the Institute of Organic Chemistry and one of the lead authors of the publication. "In contrast to the prediction of properties of individual compounds, a reaction is the interaction of many molecules and thus a multidimensional problem," he adds. Moreover, there are no clearly defined "rules of the game" which, as in the case of modern chess computers, simplify the development of AI models. For this reason, previous approaches to accurately predicting reaction results such as yields or products are mostly based on a previously gained understanding of molecular properties. "The development of such models involves a great deal of effort. Moreover, the majority of them are highly specialized and cannot be transferred to other problems," Frederik Sandfort adds.

The focus of the work presented was therefore on a general applicability of the programme, so that other chemists can easily use it for their own work. To ensure this, the model is based directly on molecular structures. "Every organic compound can be represented as a graph, in principle as an image," explains Marius Kühnemund, another author, from the field of computer science. "On such graphs, simple structural queries—comparable to the question of colours or shapes in a photo—can be made in order to capture the so-called chemical environment as accurately as possible."

The combination of many such successive queries results in a so-called molecular fingerprint. These simple number sequences have long been used in chemoinformatics to find structural similarities and are well suited for computer-aided applications. In their approach, the authors use a large number of such fingerprints to represent the chemical structure of each molecule as accurately as possible. "In this way, we have been able to develop a robust system that can be used to predict completely different reaction results," adds Marius Kühnemund, "The same model can be used to predict both yields and stereoselectivities, which is unique."

The authors demonstrated that their programme can be applied easily and allows accurate predictions, especially in combination with modern robotics, by using a data set that was not originally created for machine learning. "This data set contains only relative sales of the starting materials and no exact yields," Frederik Sandfort explains. "For exact yields, calibrations have to be created. However, due to the high effort involved, this is rarely done in reality."

The team will continue to develop their programme further and equip it with new functions in the future. Prof. Frank Glorius is confident: "When it comes to evaluating large amounts of complex data, computers are fundamentally superior to us. However, our goal is not to replace synthetic chemists with machines, but to support them as effectively as possible. Models based on artificial intelligence can significantly change the way we approach chemical syntheses. But we are still at the very beginning." [26]

Researchers review the rapid progress in machine learning for the chemical sciences

A new tool is drastically changing the face of chemical research – artificial intelligence. In a new paper published in *Nature*, researchers review the rapid progress in machine learning for the chemical sciences.

Almost every technological advance in human history is accompanied by the discovery or development of new materials, from the blending of copper and zinc to form bronze to the fabrication of high-quality silicon microchips that power digital technology.

Designing materials for a specific demand is a mind-boggling task; a random mix-and-match of atomic building blocks could yield any one of an infinite number of possible compounds. Historically, the discovery of materials has involved a combination of chance, intuition, and trial and error—but this could all be set to change thanks to artificial intelligence.

An international team of scientists from the UK and the USA, including Ph.D. student Daniel Davies from the Centre for Sustainable Chemical Technologies and Department of Chemistry, published a review on the growing potential of machine learning for chemical design.

Daniel said: "Machine learning is a branch of artificial intelligence where computers are programmed by learning from data. These methods have been around for a while, used extensively by Google, Yahoo, Amazon etc, for targeted advertising, translation and spam filtering for example.

"More recently they are being used to realise self-driving car and human-like robot technology. They are only just being applied to the physical sciences in a big way and have huge implications for the role that computers take on in science. In fact, the use of 'big data' and artificial intelligence has been referred to as the fourth industrial revolution or the fourth paradigm of science. Machine learning is now being used to speed up the scientific process, designing crucial materials and molecules that we need for sustainable development, more rapidly.

"The main purpose of the article is to explain where machine learning is starting to rise to specific challenges in molecular and materials research that simply cannot be solved without it. We also identify some key barriers that need to be overcome next. For example, finding ways in which chemicals and compounds are represented to computers that only 'think' in 1s and 0s, is a big challenge.

"Our final summary is: 'As scientists embrace the inclusion of machine learning with statistically driven design in their research programmes, the number of applications is growing at an extraordinary rate. This new generation of computational science, supported by a platform of open source tools and data sharing, has the potential to revolutionise the molecular and materials discovery process.' I think this reflects the take-home message well which is that we predict this area will become an integral part of the scientific method—not just a separate area of research."

Humans have always enjoyed reasoning and intuition capabilities that far exceed those of machines. But scientists are now starting to turn to artificial intelligence driven solutions to accelerate their own materials discovery and optimisation processes.

Dr. Keith Butler from ISIS Neutron and Muon Source, lead author of the review, said: "In traditional computational approaches, the computer is little more than a calculator, employing a hard-coded algorithm provided by a human expert. By contrast, the performance of machine learning techniques improves by seeing more and more real examples."

Machine learning and artificial intelligence offer the possibility of training computers by using the properties of materials that we already know, to help identify the champion systems of the future. Artificial intelligence approaches consider all available data equally and find trends that a human researcher may miss due to bias towards a given interpretation.

But what's fuelling the progress in this field? An important driver for the explosion of artificial intelligence in chemistry is the growth of open-source databases.

"This is particularly exciting in the context of a facility like ISIS where we produce vast quantities of data, we are sitting on a data goldmine and now we are beginning to be able to leverage that," added Dr. Butler. [25]

Robot chemist discovers new molecules and reactions

A new type of artificial-intelligence-driven chemistry could revolutionise the way molecules are discovered, scientists claim.

In a new paper published today in the journal *Nature*, chemists from the University of Glasgow discuss how they have trained an artificially-intelligent organic chemical synthesis robot to automatically explore a very large number of chemical reactions.

Their 'self-driving' system, underpinned by machine learning algorithms, can find new reactions and molecules, allowing a digital-chemical data-driven approach to locating new molecules of interest, rather than being confined to a known database and the normal rules of organic synthesis.

The result could be a decreased cost for discovering new molecules for drugs, new chemical products including materials, polymers, and molecules for high tech applications like imaging.

The team demonstrated the system's potential by searching around 1000 reactions using combinations of 18 different starting chemicals. After exploring only around 100, or 10 percent, of the possible reactions, the robot was able to predict with over 80 percent accuracy which combinations of starting chemicals should be explored to create new reactions and molecules. By exploring these reactions, they discovered a range of previously unknown new molecules and reactions, with one of the reactions classed to within the top 1 percent of the most unique reactions known.

The approach was designed and developed by the team lead by Professor Leroy (Lee) Cronin, the University of Glasgow's Regius Chair of Chemistry. Professor Cronin and his team are convinced that this result will help pave the way for the digitisation of chemistry and developing new approaches to chemistry using a digital code which drives autonomous chemical robots.

Professor Cronin said: "This approach is a key step in the digitisation of chemistry, and will allow the real time searching of chemical space leading to new discoveries of drugs, interesting molecules with valuable applications, and cutting cost, time, and crucially improving safety, reducing waste, and helping chemistry enter a new digital era." [24]

The Military Just Created An AI That Learned How To Program Software

Tired of writing your own boring code for new software? Finally, there's an AI that can do it for you.

BAYOU is an deep learning tool that basically works like a search engine for coding: tell it what sort of program you want to create with a couple of keywords, and it will spit out java code that will do what you're looking for, based on its best guess.

The tool was developed by a team of computer scientists from Rice University who received funding both from the military and Google. In a study published earlier this month on the preprint server arXiv, they describe how they built BAYOU and what sorts of problems it can help programmers solve.

Basically, BAYOU read the source code for about 1500 Android apps, which comes out to 100 million lines of Java. All that code was fed through BAYOU's neural net, resulting in AI that can, yes, program other software.

If the code that BAYOU read included any sort of information about what the code does, then BAYOU also learned what those programs were *intended* to do along with how they work. This contextual information is what lets the AI write functional software based on just a couple of key words and basic information about what the programmer wants.

Computer science majors, rejoice: your homework might be about to get much easier. And teaching people how to code may become simpler and more intuitive, as they may someday use this new AI to generate examples of code or even to check their own work. Right now, BAYOU is still in the early stages, and the team behind it is still proving their technology works.

No, this is not *that moment* in which AI becomes self-replicating; BAYOU merely generates what the researchers call "sketches" of a program that are relevant to what a programmer is trying to write. These sketches still need to be pieced together into the larger work, and they may have to be tailored to the project at hand.

But even if the technology is in its infancy, this is a major step in the search for an AI programmer, a longstanding goal for computer science researchers. Other attempts to create something like BAYOU required extensive, narrow constraints to guide programmers towards the correct type of code. Because BAYOU can get to work with just a couple of keywords, it's much less time-intensive, and much easier to use overall, for the human operators. [23]

Machine learning experiment can image-match your pose

What about exploring pictures just by moving around? Lots of 11-year-olds would find this a great idea, especially if the alternative was a homework assignment on French verbs.

Welcome to Move Mirror, where you move in front of your webcam.

Google takes to the idea of making machine learning more accessible to coders and makers. The desired outcome is inspiring them to play around with this technology. Move Mirror's intent is to show computer vision techniques such as pose estimation and to do it in fun ways.

Move Mirror matches your movements to hundreds of images of people doing similar poses. "It's kind of like a magical mirror that reflects your moves with images of all kinds of human movement—from sports and dance to martial arts, acting, and beyond," says the team.

Well, you get to match your pose against a database of tens of thousands of photos. The experiment has a welcoming message that "You move and 80,000 images move with you."

Fun aside, this experiment, a collaborative effort by PAIR, Research, and Creative Lab teams at Google and friends at Use All Five, has purpose. It signals a way of life in the machine learning development community. Advances in machine learning are paraded, with hopes to engage other people with relevant interests, as all push forward research in the field.

Irene Alvarado, Creative Technologist at Google Creative Lab, said, "With Move Mirror, we're **showing** how computer vision techniques like pose estimation can be available to anyone with a computer and a webcam. We also wanted to make machine learning more accessible to coders and makers by bringing pose estimation into the browser—hopefully inspiring them to experiment with this technology."

JC Torres in *SlashGear*: "Move Mirror may seem like a frivolous, but fun, AI demo, but it does have some **positive** implications for AI."

And on that note you can **try** it out for yourself.

Move Mirror was made using PoseNet and **TensorFlow.js**. Alvarado defined the latter as "a library that runs machine learning models on-device, in your browser—which means the pose estimation happens directly in the browser, and your images are not being stored or sent to a server."

That is a good point for those who are told they have to use a webcam for any experiment. Privacy worries promptly surface. In this experiment, the images are not sent to any Google servers while the person interacts with Move Mirror. Image recognition happens locally in the person's browser

"It's definitely impressive how sophisticated machine learning can now be done just in web browsers," Torres said. "And it's definitely reassuring to know that you don't always need to send your data, much less your photos, to some computer in the cloud just to reap the benefits of AI."

How are the images matched?

Move Mirror turns to pose information to find a matching image. This involves the sites for 17 body **parts**, e.g., right shoulder, left ankle, right hip and nose. The team noted that Move Mirror does not take into account race, gender, height, body type.

Taylor Kerns, *Android Police*, explained what happens: PoseNet "recognizes the overall position of a human subject by analyzing and adding up where different parts and joints are in a photo or video. Your position is **analyzed** in real time and compared to a set of 80,000 photos. Move Mirror shows the closest match to each of your positions, stringing them together in a slideshow."

How was this Move Mirror AI experiment built? PoseNet is the pose estimation model they use; it runs in the browser using TensorFlow.js. Alvarado said, "We hope you'll play around with Move Mirror and share your experience by making a GIF."

The **article** "Move Mirror: An AI Experiment with Pose Estimation in the Browser using TensorFlow.js," is good to check out in *Medium* if you are curious in knowing all the details about their work on this. [22]

First machine learning method capable of accurate extrapolation

Understanding how a robot will react under different conditions is essential to guaranteeing its safe operation. But how do you know what will break a robot without actually damaging it? A new method developed by scientists at the Institute of Science and Technology Austria (IST Austria) and the Max Planck Institute for Intelligent Systems (MPI for Intelligent Systems) is the first machine learning method that can use observations made under safe conditions to make accurate predictions for all possible conditions governed by the same physical dynamics. Especially designed for real-life situations, their method provides simple, interpretable descriptions of the underlying physics. The researchers will present their findings tomorrow at this year's prestigious International Conference for Machine Learning (ICML).

In the past, machine learning was only capable of interpolating data—making predictions about situations that are "between" other, known situations. It was incapable of extrapolating—making predictions about situations outside of the known—because it learns to fit the known data as closely as possible locally, regardless of how it performs outside of these situations. In addition, collecting sufficient data for effective interpolation is both time- and resource-intensive, and requires data from extreme or dangerous situations. But now, Georg Martius, former ISTFELLOW and IST Austria postdoc, and since 2017 a group leader at MPI for Intelligent Systems in Tübingen, Subham S. Sahoo, a Ph.D. student also at MPI for Intelligent Systems, and Christoph Lampert, professor at IST Austria, developed a new machine learning method that addresses these problems, and is the first machine learning method to accurately extrapolate to unseen situations.

The key feature of the new method is that it strives to reveal the true dynamics of the situation: it takes in data and returns the equations that describe the underlying physics. "If you know those equations," says Georg Martius, "then you can say what will happen in all situations, even if you haven't seen them." In other words, this is what allows the method to extrapolate reliably, making it unique among machine learning methods.

The team's method sets itself apart in several other ways as well. First, the final approximations previously produced during machine learning were far too complex for a human to understand or work with. In the new method, the resulting equations are far simpler: "Our method's equations are something you would see in a textbook—simple and intuitive," says Christoph Lampert. The latter is another key difference: other machine learning methods give no insight into the relationship between conditions and results—and thus, no intuition on whether the model is even plausible. "In every other area of research, we expect models that make physical sense, that tell us why," adds Lampert. "This is what we should expect from machine learning, and what our method provides." Finally, in order to guarantee interpretability and optimize for physical situations, the team based their learning method on a different type of framework. This new design is simpler than previous methods, which in practice means that less data is needed to give the same or even better results.

And it's not all theory: "In my group, we're actually working on developing a robot that uses this type of learning. In the future, the robot would experiment with different motions, then be able to use machine learning to uncover the equations that govern its body and movement, allowing it to avoid dangerous actions or situations," adds Martius. While robots are one active area of research, the method can be used with any type of data, from biological systems to X-ray transition energies, and can also be incorporated into larger machine learning networks. [21]

Researchers are using machine learning to understand microbial relationships

The ecosystem in and around the Amazon River is the most bio-diverse in the world. But it has some competition when considering the roughly thirty feet of the human gastrointestinal (GI) tract. This microbiome—the sum total of microorganisms in a particular environment—has been the research focus of late for Carnegie Mellon Electrical and Computer Engineering (ECE) Professor Radu Marculescu.

"It turns out, the interactions that happen in the human [GI] microbiome have far more implications than we originally thought," says Marculescu. "People associate changes in the microbiome to depression, infections, even cancer, so it's sort of like a second brain for humans."

Marculescu, along with ECE Ph.D. student Chieh Lo, has developed a machine learning algorithm—called MPLasso—that uses data to infer associations and interactions between microbes in the GI microbiome. MPLasso mines medical and scientific literature from the past few decades in search of experimental data from research focused on various types of microbial interactions and associations. MPLasso pulls this disparate information into a centralized dataset that catalogs microbial interactions within the human GI tract.

Machine learning is a novel approach for this type of investigation. Marculescu's CMU-based System Level Design Group, which commits time to cyber-physical systems research, seemed like the right venue in which to tackle such a project. In doing so, he found a way to provide medical researchers and professionals with a catalog of inferred microbial interactions that can bolster the understanding of how those interactions influence and impact human health.

Until now, it's been challenging to get a good look at how microorganisms interact in the human GI tract. Marculescu knows it will still be years before advanced technologies like engineered ingestible pills and bacteria are ready for mainstream adoption, but he sees MPLasso as a major step in helping researchers better understand how the microorganisms in the human GI tract co-exist.

Marculescu says this type of information is extremely valuable for preventive medicine because it lays the groundwork for uncovering how microbial interactions translate into a person being healthy or sick. If researchers first understand what microbes are present and how they behave together, they can then start establishing cause-and-effect relationships between microbial interactions and various types of ailments.

"Researchers also observe real experimentation. They observe microbial presence at, and interactions during, various events in the body," says Marculescu. "Based on this, one can infer a network of interactions that is predictive in nature."

MPLasso has shown to be 95 percent accurate in the associations and interactions it infers in part because it addresses issues of high-dimensionality and compositionality of human microbiome data. High-dimensionality refers to the number of potential microbial associations and interactions that exist being far larger than the number of samples available in any given library of data. Compositional data provides numbers as a percentage of a whole and not as an exact measurement.

Marculescu and Lo have made MPLasso publicly available through GitHub. When researchers download it for their own use, they are also able to upload their own data to the platform. MPLasso offers a user-friendly interface for a database that continuously updates as it constantly mines newly uploaded and relevant data.

"You'll see the difference between yesterday and a few months ago because the algorithm is automatically collecting and improving your model," says Marculescu. "Your model today is better than the one two weeks ago or two months ago simply because if something has been reported that aligns with what you're looking at, the associations become that much stronger."

The human GI tract is host to what Marculescu calls "gazillions of potential problems for the human body." Since its biodiversity rivals that of the Amazon, knowing how all those living things in our GI tract interact and impact us would be a mighty useful tool. Marculescu's work will help make it so.

Read Marculescu and Lo's research paper, recently published in *PLOS Computational Biology*. [20]

Chemical synthesis with artificial intelligence: Researchers develop new computer method

In 1996, when a computer won a match against reigning world chess champion Garry Kasparov, it was nothing short of a sensation. After this breakthrough in the world of chess, the board game Go was long considered to be a bastion reserved for human players due to its complexity. But the world's best players cannot compete with the AlphaGo software. The recipe for the success of this computer program is made possible through a combination of the so-called Monte Carlo Tree

Search and deep neural networks based on machine learning and artificial intelligence. A team of researchers from the University of Muenster in Germany has now demonstrated that this combination is extremely well suited to planning chemical syntheses—so-called retrosyntheses—with unprecedented efficiency. The study has been published in the current issue of *Nature*.

Marwin Segler, the lead author of the study, says, "Retrosynthesis is the ultimate discipline in organic chemistry. Chemists need years to master it—just like with chess or Go. In addition to straightforward expertise, you also need a goodly portion of intuition and creativity for it. So far, everyone assumed that computers couldn't keep up without experts programming in tens of thousands of rules by hand. What we have shown is that the machine can, by itself, learn the rules and their applications from the literature available."

Retrosynthesis is the standard method for designing the production of chemical compounds. Going backwards mentally, the principle is that the compound is broken down into ever smaller components until the basic components have been obtained. This analysis provides the recipe, which is then used for working "forwards" in the laboratory to produce the target molecule, proceeding from the starting materials. Although easy in theory, the process presents difficulties in practice. "Just like in chess, in every step or move, you've got variety of possibilities to choose from," says Segler. "In chemistry, however, there are orders of magnitude more possible moves than in chess, and the problem is much more complex."

This is where the new method comes into play, linking up the deep neural networks with the Monte Carlo Tree Search—a constellation so promising that a large number of researchers from a variety of disciplines are working on it. The Monte Carlo Tree Search is a method for assessing moves in a game. At every move, the computer simulates numerous variants, for example, how a game of chess might end. The most promising move is then selected.

In a similar way, the computer now looks for the best possible "moves" for chemical synthesis. It is also able to learn by using deep neural networks. To this end, the computer draws on all the chemical literature ever published, which describes almost 12 million chemical reactions. Mike Preuss, an information systems specialist and co-author of the study, says, "The deep neural networks are used for predicting which reactions are possible with a certain molecule. Using the Monte Carlo Tree Search, the computer can test whether the reactions predicted really do lead to the target molecule."

The idea of using computers to plan syntheses isn't new. "The idea is actually about 60 years old." says Segler. "People thought it would be enough, as in the case of chess, to enter a large number of rules into the computer. But that didn't work. Chemistry is very complex, and in contrast to chess or Go, it can't be grasped purely logically using simple rules. Added to this is the fact that the number of publications with new reactions doubles every 10 years or so. Neither chemists nor programmers can keep up with that. We need the help of an intelligent computer." The new method is about 30 times faster than conventional programs for planning syntheses and it finds potential synthesis routes for twice as many molecules.

In a double-blind AB test, the Muenster researchers found that chemists consider these computer-generated synthesis routes to be just as good as existing tried-and-tested ones. "We hope that, using our method, chemists will not have to try out so much in the lab," Segler adds, "and that as a

result, and using fewer resources, they will be able to produce the compounds which make our high standard of living possible." [19]

Teaching machines to spot essential information in physical systems

Two physicists at ETH Zurich and the Hebrew University of Jerusalem have developed a novel machine-learning algorithm that analyses large data sets describing a physical system and extract from them the essential information needed to understand the underlying physics.

Over the past decade, machine learning has enabled groundbreaking advances in computer vision, speech recognition and translation. More recently, machine learning has also been applied to physics problems, typically for the classification of physical phases and the numerical simulation of ground states. Maciej Koch-Janusz, a researcher at the Institute for Theoretical Physics at ETH Zurich, Switzerland, and Zohar Ringel of the Hebrew University of Jerusalem, Israel, have now explored the exciting possibility of harnessing machine learning not as a numerical simulator or a "hypothesis tester," but as an integral part of the physical reasoning process.

One important step in understanding a physical system consisting of a large number of entities—for example, the atoms making up a magnetic material—is to identify among the many degrees of freedom of the system those that are most relevant for its physical behaviour. This is traditionally a step that relies heavily on human intuition and experience. But now, Koch-Janusz and Ringel demonstrate a machine-learning algorithm based on an artificial neural network that is capable of doing just that, as they report in the journal *Nature Physics*. Their algorithm takes data about a physical system without any prior knowledge about it and extracts those degrees of freedom that are most relevant to describe the system.

Technically speaking, the machine performs one of the crucial steps of one of the conceptually most profound tools of modern theoretical physics, the so-called renormalization group. The algorithm of Koch-Janusz and Ringel provides a qualitatively new approach: the internal data representations discovered by suitably designed machine-learning systems are often considered to be obscure, but the results yielded by their algorithm provide fundamental physical insight, reflecting the underlying structure of physical system. This raises the prospect of employing machine learning in science in a collaborative fashion, combining the power of machines to distil information from vast data sets with human creativity and background knowledge. [18]

Teaching computers to guide science: Machine learning method sees forests and trees

While it may be the era of supercomputers and "big data," without smart methods to mine all that data, it's only so much digital detritus. Now researchers at the Department of Energy's Lawrence

Berkeley National Laboratory (Berkeley Lab) and UC Berkeley have come up with a novel machine learning method that enables scientists to derive insights from systems of previously intractable complexity in record time.

In a paper published recently in the *Proceedings of the National Academy of Sciences* (*PNAS*), the researchers describe a technique called "iterative Random Forests," which they say could have a transformative effect on any area of science or engineering with complex systems, including biology, precision medicine, materials science, environmental science, and manufacturing, to name a few.

"Take a human cell, for example. There are 10^{170} possible molecular interactions in a single cell. That creates considerable computing challenges in searching for relationships," said Ben Brown, head of Berkeley Lab's Molecular Ecosystems Biology Department. "Our method enables the identification of interactions of high order at the same computational cost as main effects - even when those interactions are local with weak marginal effects."

Brown and Bin Yu of UC Berkeley are lead senior authors of "Iterative Random Forests to Discover Predictive and Stable High-Order Interactions." The co-first authors are Sumanta Basu (formerly a joint postdoc of Brown and Yu and now an assistant professor at Cornell University) and Karl Kumbier (a Ph.D. student of Yu in the UC Berkeley Statistics Department). The paper is the culmination of three years of work that the authors believe will transform the way science is done. "With our method we can gain radically richer information than we've ever been able to gain from a learning machine," Brown said.

The needs of machine learning in science are different from that of industry, where machine learning has been used for things like playing chess, making self-driving cars, and predicting the stock market.

"The machine learning developed by industry is great if you want to do high-frequency trading on the stock market," Brown said. "You don't care why you're able to predict the stock will go up or down. You just want to know that you can make the predictions."

But in science, questions surrounding why a process behaves in certain ways are critical. Understanding "why" allows scientists to model or even engineer processes to improve or attain a desired outcome. As a result, machine learning for science needs to peer inside the black box and understand why and how computers reached the conclusions they reached. A long-term goal is to use this kind of information to model or engineer systems to obtain desired outcomes.

In highly complex systems - whether it's a single cell, the human body, or even an entire ecosystem - there are a large number of variables interacting in nonlinear ways. That makes it difficult if not impossible to build a model that can determine cause and effect. "Unfortunately, in biology, you come across interactions of order 30, 40, 60 all the time," Brown said. "It's completely intractable with traditional approaches to statistical learning."

The method developed by the team led by Brown and Yu, iterative Random Forests (iRF), builds on an algorithm called random forests, a popular and effective predictive modeling tool, translating the internal states of the black box learner into a human-interpretable form. Their approach allows

researchers to search for complex interactions by decoupling the order, or size, of interactions from the computational cost of identification.

"There is no difference in the computational cost of detecting an interaction of order 30 versus an interaction of order two," Brown said. "And that's a sea change."

In the PNAS paper, the scientists demonstrated their method on two genomics problems, the role of gene enhancers in the fruit fly embryo and alternative splicing in a human-derived cell line. In both cases, using iRF confirmed previous findings while also uncovering previously unidentified higher-order interactions for follow-up study.

Brown said they're now using their method for designing phased array laser systems and optimizing sustainable agriculture systems.

"We believe this is a different paradigm for doing science," said Yu, a professor in the departments of Statistics and Electrical Engineering & Computer Science at UC Berkeley. "We do prediction, but we introduce stability on top of prediction in iRF to more reliably learn the underlying structure in the predictors."

"This enables us to learn how to engineer systems for goal-oriented optimization and more accurately targeted simulations and follow-up experiments," Brown added.

In a PNAS commentary on the technique, Danielle Denisko and Michael Hoffman of the University of Toronto wrote: "iRF holds much promise as a new and effective way of detecting interactions in a variety of settings, and its use will help us ensure no branch or leaf is ever left unturned." [17]

Rise of the quantum thinking machines

Quantum computers can be made to utilize effects such as quantum coherence and entanglement to accelerate machine learning.

Although we typically view information as being an abstract or virtual entity, information, of course, must be stored in a physical medium. Information processing devices such as computers and phones are therefore fundamentally governed by the laws of physics. In this way, the fundamental physical limits of an agent's ability to learn are governed by the laws of physics. The best known theory of physics is quantum theory, which ultimately must be used to determine the absolute physical limits of a machine's ability to learn.

A quantum algorithm is a stepwise procedure performed on a quantum computer to solve a problem such as searching a database. Quantum machine learning software makes use of quantum algorithms to process information in ways that classical computers cannot. These quantum effects open up exciting new avenues which can, in principle, outperform the best known classical algorithms when solving certain machine learning problems. This is known as quantum enhanced machine learning.

Machine learning methods use mathematical algorithms to search for certain patterns in large data sets. Machine learning is widely used in biotechnology, pharmaceuticals, particle physics and many other fields. Thanks to the ability to adapt to new data, machine learning greatly exceeds the ability of people. Despite this, machine learning cannot cope with certain difficult tasks.

Quantum enhancement is predicted to be possible for a host of machine learning tasks, ranging from optimization to quantum enhanced deep learning.

In the new paper published in Nature, a group of scientists led by Skoltech Associate Professor Jacob Biamonte produced a feasibility analysis outlining what steps can be taken for practical quantum enhanced machine learning.

The prospects of using quantum computers to accelerate machine learning has generated recent excitement due to the increasing capabilities of quantum computers. This includes a commercially available 2000 spin quantum accelerated annealing by the Canada-based company D-Wave Systems Inc. and a 16 qubit universal quantum processor by IBM which is accessible via a (currently free) cloud service.

The availability of these devices has led to increased interest from the machine learning community. The interest comes as a bit of a shock to the traditional quantum physics community, in which researchers have thought that the primary applications of quantum computers would be using quantum computers to simulate chemical physics, which can be used in the pharmaceutical industry for drug discovery. However, certain quantum systems can be mapped to certain machine learning models, particularly deep learning models. Quantum machine learning can be used to work in tandem with these existing methods for quantum chemical emulation, leading to even greater capabilities for a new era of quantum technology.

"Early on, the team burned the midnight oil over Skype, debating what the field even was—our synthesis will hopefully solidify topical importance. We submitted our draft to Nature, going forward subject to significant changes. All in all, we ended up writing three versions over eight months with nothing more than the title in common," said lead study author Biamonte. [16]

A Machine Learning Systems That Called Neural Networks Perform Tasks by Analyzing Huge Volumes of Data

Neural networks learn how to carry out certain tasks by analyzing large amounts of data displayed to them. These machine learning systems continually learn and readjust to be able to carry out the task set out before them. Understanding how neural networks work helps researchers to develop better applications and uses for them.

At the 2017 Conference on Empirical Methods on Natural Language Processing earlier this month, MIT researchers demonstrated a new general-purpose technique for making sense of neural networks that are able to carry out natural language processing tasks where they attempt to extract data written in normal text opposed to something of a structured language like database-query language.

The new technique works great in any system that reads the text as input and produces symbols as the output. One such example of this can be seen in an automatic translator. It works without the need to access any underlying software too. Tommi Jaakkola is Professor of Electrical Engineering and Computer Science at MIT and one of the authors on the paper. He says, "I can't just do a simple randomization. And what you are predicting is now a more complex object, like a sentence, so what does it mean to give an explanation?"

As part of the research, Jaakkola, and colleague David Alvarez-Melis, an MIT graduate student in electrical engineering and computer science and first author on the paper, used a black-box neural net in which to generate test sentences to feed black-box neural nets. The duo began by teaching the network to compress and decompress natural sentences. As the training continues the encoder and decoder get evaluated simultaneously depending on how closely the decoder's output matches up with the encoder's input.

Neural nets work on probabilities. For example, an object-recognition system could be fed an image of a cat, and it would process that image as it saying 75 percent probability of being a cat, while still having a 25 percent probability that it's a dog. Along with that same line, Jaakkola and Alvarez-Melis' sentence compressing network has alternative words for each of those in a decoded sentence along with the probability that each is correct. So, once the system has generated a list of closely related sentences they're then fed to a black-box natural language processor. This then allows the researchers to analyze and determine which inputs have an effect on which outputs.

During the research, the pair applied this technique to three different types of a natural language processing system. The first one inferred the way in which words were pronounced; the second was a set of translators, and the third was a simple computer dialogue system which tried to provide adequate responses to questions or remarks. In looking at the results, it was clear and pretty obvious that the translation systems had strong dependencies on individual words of both the input and output sentences. A little more surprising, however, was the identification of gender biases in the texts on which the machine translation systems were trained. The dialogue system was too small to take advantage of the training set.

"The other experiment we do is in flawed systems," says Alvarez-Melis. "If you have a black-box model that is not doing a good job, can you first use this kind of approach to identify problems? A motivating application of this kind of interpretability is to fix systems, to improve systems, by understanding what they're getting wrong and why." [15]

Active machine learning for the discovery and crystallization of gigantic polyoxometalate molecules

Who is the better experimentalist, a human or a robot? When it comes to exploring synthetic and crystallization conditions for inorganic gigantic molecules, actively learning machines are clearly ahead, as demonstrated by British Scientists in an experiment with polyoxometalates published in the journal Angewandte Chemie.

Polyoxometalates form through self-assembly of a large number of metal atoms bridged by oxygen atoms. Potential uses include catalysis, electronics, and medicine. Insights into the self-

organization processes could also be of use in developing functional chemical systems like "molecular machines".

Polyoxometalates offer a nearly unlimited variety of structures. However, it is not easy to find new ones, because the aggregation of complex inorganic molecules to gigantic molecules is a process that is difficult to predict. It is necessary to find conditions under which the building blocks aggregate and then also crystallize, so that they can be characterized.

A team led by Leroy Cronin at the University of Glasgow (UK) has now developed a new approach to define the range of suitable conditions for the synthesis and crystallization of polyoxometalates. It is based on recent advances in machine learning, known as active learning. They allowed their trained machine to compete against the intuition of experienced experimenters. The test example was Na(6)[Mo(120)Ce(6)O(366)H(12)(H(2)O)(78)]·200 H(2)O, a new, ring-shaped polyoxometalate cluster that was recently discovered by the researchers' automated chemical robot.

In the experiment, the relative quantities of the three necessary reagent solutions were to be varied while the protocol was otherwise prescribed. The starting point was a set of data from successful and unsuccessful crystallization experiments. The aim was to plan ten experiments and then use the results from these to proceed to the next set of ten experiments - a total of one hundred crystallization attempts.

Although the flesh-and-blood experimenters were able to produce more successful crystallizations, the far more "adventurous" machine algorithm was superior on balance because it covered a significantly broader domain of the "crystallization space". The quality of the prediction of whether an experiment would lead to crystallization was improved significantly more by the machine than the human experimenters. A series of 100 purely random experiments resulted in no improvement. In addition, the machine discovered a range of conditions that led to crystals which would not have been expected based on pure intuition. This "unbiased" automated method makes the discovery of novel compounds more probably than reliance on human intuition. The researchers are now looking for ways to make especially efficient "teams" of man and machine. [14]

Using machine learning to understand materials

Whether you realize it or not, machine learning is making your online experience more efficient. The technology, designed by computer scientists, is used to better understand, analyze, and categorize data. When you tag your friend on Facebook, clear your spam filter, or click on a suggested YouTube video, you're benefitting from machine learning algorithms.

Machine learning algorithms are designed to improve as they encounter more data, making them a versatile technology for understanding large sets of photos such as those accessible from Google Images. Elizabeth Holm, professor of materials science and engineering at Carnegie Mellon University, is leveraging this technology to better understand the enormous number of research images accumulated in the field of materials science. This unique application is an interdisciplinary approach to machine learning that hasn't been explored before.

"Just like you might search for cute cat pictures on the internet, or Facebook recognizes the faces of your friends, we are creating a system that allows a computer to automatically understand the visual data of materials science," explains Holm.

The field of materials science usually relies on human experts to identify research images by hand. Using machine learning algorithms, Holm and her group have created a system that automatically recognizes and categorizes microstructural images of materials. Her goal is to make it more efficient for materials scientists to search, sort, classify, and identify important information in their visual data.

"In materials science, one of our fundamental data is pictures," explains Holm. "Images contain information that we recognize, even when we find it difficult to quantify numerically."

Holm's machine learning system has several different applications within the materials science field including research, industry, publishing, and academia. For example, the system could be used to create a visual search of a scientific journal archives so that a researcher could find out whether a similar image had ever been published. Similarly, the system can be used to automatically search and categorize image archives in industries or research labs. "Big companies can have archives of 600,000 or more research images. No one wants to look through those, but they want to use that data to better understand their products," explains Holm. "This system has the power to unlock those archives."

Holm and her group have been working on this research for about three years and are continuing to grow the project, especially as it relates to the metal 3-D printing field. For example, they are beginning to compile a database of experimental and simulated metal powder micrographs in order to better understand what types of raw materials are best suited for 3-D printing processes.

Holm published an article about this research in the December 2015 issue of Computational Materials Science titled "A computer vision approach for automated analysis and classification of microstructural image data." [13]

Artificial intelligence helps in the discovery of new materials

With the help of artificial intelligence, chemists from the University of Basel in Switzerland have computed the characteristics of about two million crystals made up of four chemical elements. The researchers were able to identify 90 previously unknown thermodynamically stable crystals that can be regarded as new materials.

They report on their findings in the scientific journal Physical Review Letters.

Elpasolite is a glassy, transparent, shiny and soft mineral with a cubic crystal structure. First discovered in El Paso County (Colorado, USA), it can also be found in the Rocky Mountains, Virginia and the Apennines (Italy). In experimental databases, elpasolite is one of the most frequently found quaternary crystals (crystals made up of four chemical elements). Depending on its composition, it can be a metallic conductor, a semi-conductor or an insulator, and may also emit light when exposed to radiation.

These characteristics make elpasolite an interesting candidate for use in scintillators (certain aspects of which can already be demonstrated) and other applications. Its chemical complexity means that, mathematically speaking, it is practically impossible to use quantum mechanics to predict every theoretically viable combination of the four elements in the structure of elpasolite.

Machine learning aids statistical analysis

Thanks to modern artificial intelligence, Felix Faber, a doctoral student in Prof. Anatole von Lilienfeld's group at the University of Basel's Department of Chemistry, has now succeeded in solving this material design problem. First, using quantum mechanics, he generated predictions for thousands of elpasolite crystals with randomly determined chemical compositions. He then used the results to train statistical machine learning models (ML models). The improved algorithmic strategy achieved a predictive accuracy equivalent to that of standard quantum mechanical approaches.

ML models have the advantage of being several orders of magnitude quicker than corresponding quantum mechanical calculations. Within a day, the ML model was able to predict the formation energy – an indicator of chemical stability – of all two million elpasolite crystals that theoretically can be obtained from the main group elements of the periodic table. In contrast, performance of the calculations by quantum mechanical means would have taken a supercomputer more than 20 million hours.

Unknown materials with interesting characteristics

An analysis of the characteristics computed by the model offers new insights into this class of materials. The researchers were able to detect basic trends in formation energy and identify 90 previously unknown crystals that should be thermodynamically stable, according to quantum mechanical predictions.

On the basis of these potential characteristics, elpasolite has been entered into the Materials Project material database, which plays a key role in the Materials Genome Initiative. The initiative was launched by the US government in 2011 with the aim of using computational support to accelerate the discovery and the experimental synthesis of interesting new materials.

Some of the newly discovered elpasolite crystals display exotic electronic characteristics and unusual compositions. "The combination of artificial intelligence, big data, quantum mechanics and supercomputing opens up promising new avenues for deepening our understanding of materials and discovering new ones that we would not consider if we relied solely on human intuition," says study director von Lilienfeld. [12]

Physicists are putting themselves out of a job, using artificial intelligence to run a complex experiment

The experiment, developed by physicists from The Australian National University (ANU) and UNSW ADFA, created an extremely cold gas trapped in a laser beam, known as a Bose-Einstein condensate, replicating the experiment that won the 2001 Nobel Prize.

"I didn't expect the machine could learn to do the experiment itself, from scratch, in under an hour," said co-lead researcher Paul Wigley from the ANU Research School of Physics and Engineering.

"A simple computer program would have taken longer than the age of the Universe to run through all the combinations and work this out."

Bose-Einstein condensates are some of the coldest places in the Universe, far colder than outer space, typically less than a billionth of a degree above absolute zero.

They could be used for mineral exploration or navigation systems as they are extremely sensitive to external disturbances, which allows them to make very precise measurements such as tiny changes in the Earth's magnetic field or gravity.

The artificial intelligence system's ability to set itself up quickly every morning and compensate for any overnight fluctuations would make this fragile technology much more useful for field measurements, said co-lead researcher Dr Michael Hush from UNSW ADFA.

"You could make a working device to measure gravity that you could take in the back of a car, and the artificial intelligence would recalibrate and fix itself no matter what," he said.

"It's cheaper than taking a physicist everywhere with you."

The team cooled the gas to around 1 microkelvin, and then handed control of the three laser beams over to the artificial intelligence to cool the trapped gas down to nanokelvin.

Researchers were surprised by the methods the system came up with to ramp down the power of the lasers.

"It did things a person wouldn't guess, such as changing one laser's power up and down, and compensating with another," said Mr Wigley.

"It may be able to come up with complicated ways humans haven't thought of to get experiments colder and make measurements more precise.

The new technique will lead to bigger and better experiments, said Dr Hush.

"Next we plan to employ the artificial intelligence to build an even larger Bose-Einstein condensate faster than we've seen ever before," he said.

The research is published in the Nature group journal Scientific Reports. [11]

Quantum experiments designed by machines

The idea was developed when the physicists wanted to create new quantum states in the laboratory, but were unable to conceive of methods to do so. "After many unsuccessful attempts to come up with an experimental implementation, we came to the conclusion that our intuition about these phenomena seems to be wrong. We realized that in the end we were just trying random arrangements of quantum building blocks. And that is what a computer can do as well -

but thousands of times faster", explains Mario Krenn, PhD student in Anton Zeilinger's group and first author research.

After a few hours of calculation, their algorithm - which they call Melvin - found the recipe to the question they were unable to solve, and its structure surprised them. Zeilinger says: "Suppose I want build an experiment realizing a specific quantum state I am interested in. Then humans intuitively consider setups reflecting the symmetries of the state. Yet Melvin found out that the most simple realization can be asymmetric and therefore counterintuitive. A human would probably never come up with that solution."

The physicists applied the idea to several other questions and got dozens of new and surprising answers. "The solutions are difficult to understand, but we were able to extract some new experimental tricks we have not thought of before. Some of these computer-designed experiments are being built at the moment in our laboratories", says Krenn.

Melvin not only tries random arrangements of experimental components, but also learns from previous successful attempts, which significantly speeds up the discovery rate for more complex solutions. In the future, the authors want to apply their algorithm to even more general questions in quantum physics, and hope it helps to investigate new phenomena in laboratories. [10]

Moving electrons around loops with light: A quantum device based on geometry

Researchers at the University of Chicago's Institute for Molecular Engineering and the University of Konstanz have demonstrated the ability to generate a quantum logic operation, or rotation of the qubit, that - surprisingly—is intrinsically resilient to noise as well as to variations in the strength or duration of the control. Their achievement is based on a geometric concept known as the Berry phase and is implemented through entirely optical means within a single electronic spin in diamond.

Their findings were published online Feb. 15, 2016, in Nature Photonics and will appear in the March print issue. "We tend to view quantum operations as very fragile and susceptible to noise, especially when compared to conventional electronics," remarked David Awschalom, the Liew Family Professor of Molecular Engineering and senior scientist at Argonne National Laboratory, who led the research. "In contrast, our approach shows incredible resilience to external influences and fulfills a key requirement for any practical quantum technology."

Quantum geometry

When a quantum mechanical object, such as an electron, is cycled along some loop, it retains a memory of the path that it travelled, the Berry phase. To better understand this concept, the Foucault pendulum, a common staple of science museums helps to give some intuition. A pendulum, like those in a grandfather clock, typically oscillates back and forth within a fixed plane. However, a Foucault pendulum oscillates along a plane that gradually rotates over the course of a day due to Earth's rotation, and in turn knocks over a series of pins encircling the pendulum.

The number of knocked-over pins is a direct measure of the total angular shift of the pendulum's oscillation plane, its acquired geometric phase. Essentially, this shift is directly related to the

location of the pendulum on Earth's surface as the rotation of Earth transports the pendulum along a specific closed path, its circle of latitude. While this angular shift depends on the particular path traveled, Awschalom said, it remarkably does not depend on the rotational speed of Earth or the oscillation frequency of the pendulum.

"Likewise, the Berry phase is a similar path-dependent rotation of the internal state of a quantum system, and it shows promise in quantum information processing as a robust means to manipulate qubit states," he said.

A light touch

In this experiment, the researchers manipulated the Berry phase of a quantum state within a nitrogen-vacancy (NV) center, an atomic-scale defect in diamond. Over the past decade and a half, its electronic spin state has garnered great interest as a potential qubit. In their experiments, the team members developed a method with which to draw paths for this defect's spin by varying the applied laser light. To demonstrate Berry phase, they traced loops similar to that of a tangerine slice within the quantum space of all of the potential combinations of spin states.

"Essentially, the area of the tangerine slice's peel that we drew dictated the amount of Berry phase that we were able to accumulate," said Christopher Yale, a postdoctoral scholar in Awschalom's laboratory, and one of the co-lead authors of the project.

This approach using laser light to fully control the path of the electronic spin is in contrast to more common techniques that control the NV center spin, through the application of microwave fields. Such an approach may one day be useful in developing photonic networks of these defects, linked and controlled entirely by light, as a way to both process and transmit quantum information.

A noisy path

A key feature of Berry phase that makes it a robust quantum logic operation is its resilience to noise sources. To test the robustness of their Berry phase operations, the researchers intentionally added noise to the laser light controlling the path. As a result, the spin state would travel along its intended path in an erratic fashion.

However, as long as the total area of the path remained the same, so did the Berry phase that they measured.

"In particular, we found the Berry phase to be insensitive to fluctuations in the intensity of the laser. Noise like this is normally a bane for quantum control," said Brian Zhou, a postdoctoral scholar in the group, and co-lead author.

"Imagine you're hiking along the shore of a lake, and even though you continually leave the path to go take pictures, you eventually finish hiking around the lake," said F. Joseph Heremans, co-lead author, and now a staff scientist at Argonne National Laboratory. "You've still hiked the entire loop regardless of the bizarre path you took, and so the area enclosed remains virtually the same."

These optically controlled Berry phases within diamond suggest a route toward robust and faulttolerant quantum information processing, noted Guido Burkard, professor of physics at the University of Konstanz and theory collaborator on the project.

"Though its technological applications are still nascent, Berry phases have a rich underlying mathematical framework that makes them a fascinating area of study," Burkard said. [9]

Researchers demonstrate 'quantum surrealism'

In a new version of an old experiment, CIFAR Senior Fellow Aephraim Steinberg (University of Toronto) and colleagues tracked the trajectories of photons as the particles traced a path through one of two slits and onto a screen. But the researchers went further, and observed the "nonlocal" influence of another photon that the first photon had been entangled with.

The results counter a long-standing criticism of an interpretation of quantum mechanics called the De Broglie-Bohm theory. Detractors of this interpretation had faulted it for failing to explain the behaviour of entangled photons realistically. For Steinberg, the results are important because they give us a way of visualizing quantum mechanics that's just as valid as the standard interpretation, and perhaps more intuitive.

"I'm less interested in focusing on the philosophical question of what's 'really' out there. I think the fruitful question is more down to earth. Rather than thinking about different metaphysical interpretations, I would phrase it in terms of having different pictures. Different pictures can be useful. They can help shape better intuitions."

At stake is what is "really" happening at the quantum level. The uncertainty principle tells us that we can never know both a particle's position and momentum with complete certainty. And when we do interact with a quantum system, for instance by measuring it, we disturb the system. So if we fire a photon at a screen and want to know where it will hit, we'll never know for sure exactly where it will hit or what path it will take to get there.

The standard interpretation of quantum mechanics holds that this uncertainty means that there is no "real" trajectory between the light source and the screen. The best we can do is to calculate a "wave function" that shows the odds of the photon being in any one place at any time, but won't tell us where it is until we make a measurement.

Yet another interpretation, called the De Broglie-Bohm theory, says that the photons do have real trajectories that are guided by a "pilot wave" that accompanies the particle. The wave is still probabilistic, but the particle takes a real trajectory from source to target. It doesn't simply "collapse" into a particular location once it's measured.

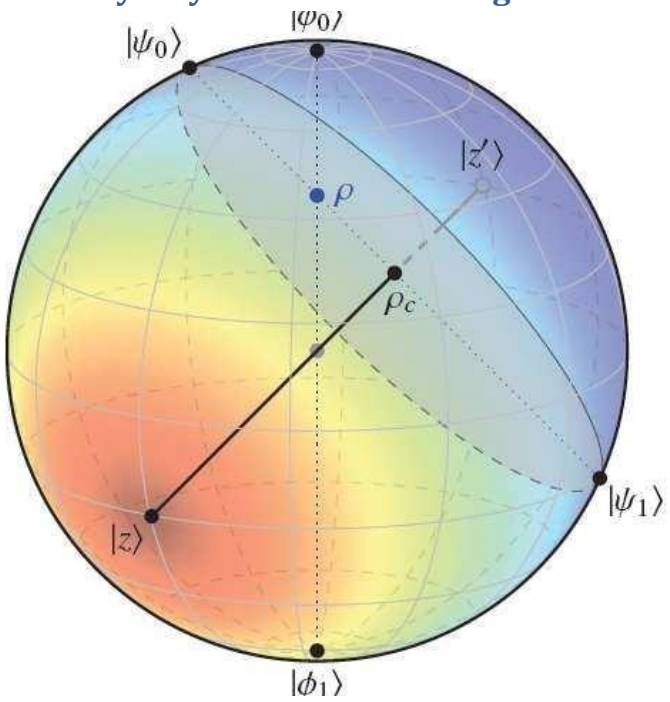
In 2011 Steinberg and his colleagues showed that they could follow trajectories for photons by subjecting many identical particles to measurements so weak that the particles were barely disturbed, and then averaging out the information. This method showed trajectories that looked similar to classical ones - say, those of balls flying through the air.

But critics had pointed out a problem with this viewpoint. Quantum mechanics also tells us that two particles can be entangled, so that a measurement of one particle affects the other. The critics complained that in some cases, a measurement of one particle would lead to an incorrect prediction of the trajectory of the entangled particle. They coined the term "surreal trajectories" to describe them.

In the most recent experiment, Steinberg and colleagues showed that the surrealism was a consequence of non-locality - the fact that the particles were able to influence one another instantaneously at a distance. In fact, the "incorrect" predictions of trajectories by the entangled photon were actually a consequence of where in their course the entangled particles were measured. Considering both particles together, the measurements made sense and were consistent with real trajectories.

Steinberg points out that both the standard interpretation of quantum mechanics and the De Broglie-Bohm interpretation are consistent with experimental evidence, and are mathematically equivalent. But it is helpful in some circumstances to visualize real trajectories, rather than wave function collapses, he says. [8]

Physicists discover easy way to measure entanglement—on a sphere



Entanglement on a sphere: This Bloch sphere shows entanglement for the one-root state ρ and its radial state ρc. The color on the sphere corresponds to the value of the entanglement, which is determined by the distance from the root state z, the point at which there is no entanglement. The closer to z, the less the entanglement (red); the further from z, the greater the entanglement (blue). Credit: Regula and Adesso. ©2016 American Physical Society

Now in a new paper to be published in Physical Review Letters, mathematical physicists Bartosz Regula and Gerardo Adesso at The University of Nottingham have greatly simplified the problem of measuring entanglement.

To do this, the scientists turned the difficult analytical problem into an easy geometrical one. They showed that, in many cases, the amount of entanglement between states corresponds to the distance between two points on a Bloch sphere, which is basically a normal 3D sphere that physicists use to model quantum states.

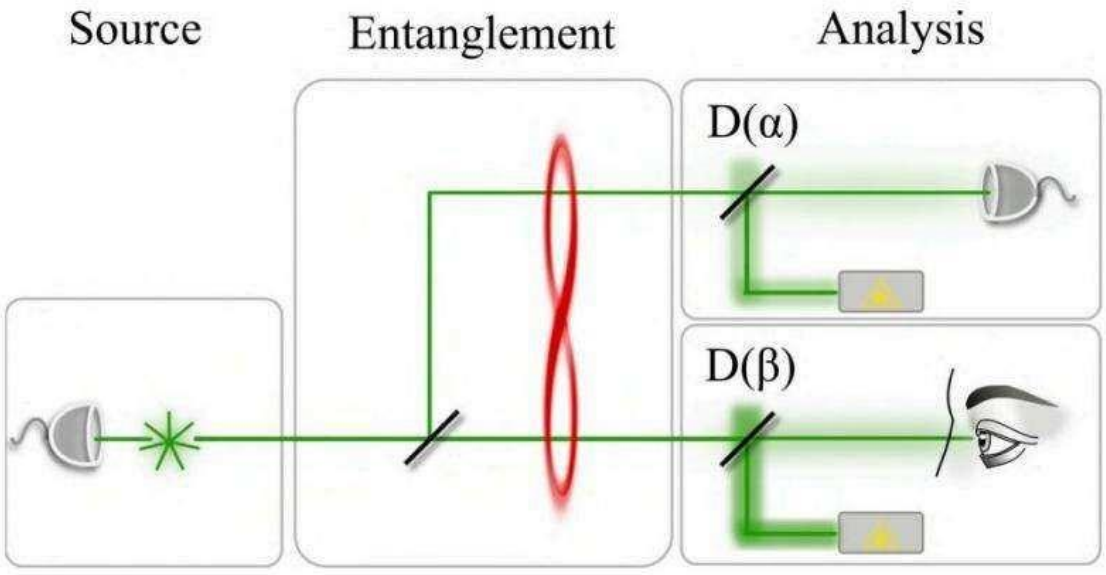
As the scientists explain, the traditionally difficult part of the math problem is that it requires finding the optimal decomposition of mixed states into pure states. The geometrical approach completely eliminates this requirement by reducing the many possible ways that states could decompose down to a single point on the sphere at which there is zero entanglement. The approach requires that there be only one such point, or "root," of zero entanglement, prompting the physicists to describe the method as "one root to rule them all."

The scientists explain that the "one root" property is common among quantum states and can be easily verified, transforming a formidable math problem into one that is trivially easy. They demonstrated that the new approach works for many types of two-, three- and four-qubit entangled states.

"This method reveals an intriguing and previously unexplored connection between the quantum features of a state and classical geometry, allowing all one-root states to enjoy a convenient visual representation which considerably simplifies the study and understanding of their properties," the researchers explained.

The simple way of measuring a state's entanglement could have applications in many technological areas, such as quantum cryptography, computation, and communication. It could also provide insight into understanding the foundations of thermodynamics, condensed matter physics, and biology. [7]

An idea for allowing the human eye to observe an instance of entanglement



Scheme of the proposal for detecting entanglement with the human eye. Credit: arXiv:1602.01907

Entanglement, is of course, where two quantum particles are intrinsically linked to the extent that they actually share the same existence, even though they can be separated and moved apart. The idea was first proposed nearly a century ago, and it has not only been proven, but researchers

routinely cause it to occur, but, to date, not one single person has every actually seen it happen—they only know it happens by conducting a series of experiments. It is not clear if anyone has ever actually tried to see it happen, but in this new effort, the research trio claim to have found a way to make it happen—if only someone else will carry out the experiment on a willing volunteer.

The idea involves using a beam splitter and two beans of light—an initial beam of coherent photons fired at the beam splitter and a secondary beam of coherent photons that interferes with the photons in the first beam causing a change of phase, forcing the light to be reflected rather than transmitted. In such a scenario, the secondary beam would not need to be as intense as the first, and could in fact be just a single coherent photon—if it were entangled, it could be used to allow a person to see the more powerful beam while still preserving the entanglement of the original photon.

The researchers suggest the technology to carry out such an experiment exists today, but also acknowledge that it would take a special person to volunteer for such an assignment because to prove that they had seen entanglement taking place would involve shooting a large number of photons in series, into a person's eye, whereby the resolute volunteer would announce whether they had seen the light on the order of thousands of times. [6]

Quantum entanglement

Measurements of physical properties such as position, momentum, spin, polarization, etc. performed on entangled particles are found to be appropriately correlated. For example, if a pair of particles is generated in such a way that their total spin is known to be zero, and one particle is found to have clockwise spin on a certain axis, then the spin of the other particle, measured on the same axis, will be found to be counterclockwise. Because of the nature of quantum measurement, however, this behavior gives rise to effects that can appear paradoxical: any measurement of a property of a particle can be seen as acting on that particle (e.g. by collapsing a number of superimposed states); and in the case of entangled particles, such action must be on the entangled system as a whole. It thus appears that one particle of an entangled pair "knows" what measurement has been performed on the other, and with what outcome, even though there is no known means for such information to be communicated between the particles, which at the time of measurement may be separated by arbitrarily large distances. [4]

The Bridge

The accelerating electrons explain not only the Maxwell Equations and the Special Relativity, but the Heisenberg Uncertainty Relation, the wave particle duality and the electron’s spin also, building the bridge between the Classical and Quantum Theories. [1]

Accelerating charges

The moving charges are self maintain the electromagnetic field locally, causing their movement and this is the result of their acceleration under the force of this field. In the classical physics the charges will distributed along the electric current so that the electric potential lowering along the

current, by linearly increasing the way they take every next time period because this accelerated motion. The same thing happens on the atomic scale giving a dp impulse difference and a dx way difference between the different part of the not point like particles.

Relativistic effect

Another bridge between the classical and quantum mechanics in the realm of relativity is that the charge distribution is lowering in the reference frame of the accelerating charges linearly: $ds/dt = at$ (time coordinate), but in the reference frame of the current it is parabolic: $s = a/2\ t^2$ (geometric coordinate).

Heisenberg Uncertainty Relation

In the atomic scale the Heisenberg uncertainty relation gives the same result, since the moving electron in the atom accelerating in the electric field of the proton, causing a charge distribution on delta x position difference and with a delta p momentum difference such a way that they product is about the half Planck reduced constant. For the proton this delta x much less in the nucleon, than in the orbit of the electron in the atom, the delta p is much higher because of the greater proton mass.

This means that the electron and proton are not point like particles, but has a real charge distribution.

Wave – Particle Duality

The accelerating electrons explains the wave – particle duality of the electrons and photons, since the elementary charges are distributed on delta x position with delta p impulse and creating a wave packet of the electron. The photon gives the electromagnetic particle of the mediating force of the electrons electromagnetic field with the same distribution of wavelengths.

Atomic model

The constantly accelerating electron in the Hydrogen atom is moving on the equipotential line of the proton and it's kinetic and potential energy will be constant. Its energy will change only when it is changing its way to another equipotential line with another value of potential energy or getting free with enough kinetic energy. This means that the Rutherford-Bohr atomic model is right and only that changing acceleration of the electric charge causes radiation, not the steady acceleration. The steady acceleration of the charges only creates a centric parabolic steady electric field around the charge, the magnetic field. This gives the magnetic moment of the atoms, summing up the proton and electron magnetic moments caused by their circular motions and spins.

The Relativistic Bridge

Commonly accepted idea that the relativistic effect on the particle physics it is the fermions' spin - another unresolved problem in the classical concepts. If the electric charges can move only with accelerated motions in the self maintaining electromagnetic field, once upon a time they would reach the velocity of the electromagnetic field. The resolution of this problem is the spinning particle, constantly accelerating and not reaching the velocity of light because the acceleration is radial. One origin of the Quantum Physics is the Planck Distribution Law of the electromagnetic oscillators, giving equal intensity for 2 different wavelengths on any temperature. Any of these two wavelengths will give equal intensity diffraction patterns, building different asymmetric constructions, for example proton - electron structures (atoms), molecules, etc. Since the particles are centers of diffraction patterns they also have particle – wave duality as the electromagnetic waves have. [2]

The weak interaction

The weak interaction transforms an electric charge in the diffraction pattern from one side to the other side, causing an electric dipole momentum change, which violates the CP and time reversal symmetry. The Electroweak Interaction shows that the Weak Interaction is basically electromagnetic in nature. The arrow of time shows the entropy grows by changing the temperature dependent diffraction patterns of the electromagnetic oscillators.

Another important issue of the quark model is when one quark changes its flavor such that a linear oscillation transforms into plane oscillation or vice versa, changing the charge value with 1 or -1. This kind of change in the oscillation mode requires not only parity change, but also charge and time changes (CPT symmetry) resulting a right handed anti-neutrino or a left handed neutrino.

The right handed anti-neutrino and the left handed neutrino exist only because changing back the quark flavor could happen only in reverse, because they are different geometrical constructions, the u is 2 dimensional and positively charged and the d is 1 dimensional and negatively charged. It needs also a time reversal, because anti particle (anti neutrino) is involved.

The neutrino is a 1/2spin creator particle to make equal the spins of the weak interaction, for example neutron decay to 2 fermions, every particle is fermions with ½ spin. The weak interaction changes the entropy since more or less particles will give more or less freedom of movement. The entropy change is a result of temperature change and breaks the equality of oscillator diffraction intensity of the Maxwell–Boltzmann statistics. This way it changes the time coordinate measure and
makes possible a different time dilation as of the special relativity.

The limit of the velocity of particles as the speed of light appropriate only for electrical charged particles, since the accelerated charges are self maintaining locally the accelerating electric force. The neutrinos are CP symmetry breaking particles compensated by time in the CPT symmetry, that is the time coordinate not works as in the electromagnetic interactions, consequently the speed of neutrinos is not limited by the speed of light.

The weak interaction T-asymmetry is in conjunction with the T-asymmetry of the second law of thermodynamics, meaning that locally lowering entropy (on extremely high temperature) causes the
weak interaction, for example the Hydrogen fusion.

Probably because it is a spin creating movement changing linear oscillation to 2 dimensional oscillation by changing d to u quark and creating anti neutrino going back in time relative to the proton and electron created from the neutron, it seems that the anti neutrino fastest then the velocity of the photons created also in this weak interaction?

A quark flavor changing shows that it is a reflection changes movement and the CP- and T-symmetry breaking!!! This flavor changing oscillation could prove that it could be also on higher level such as atoms, molecules, probably big biological significant molecules and responsible on the aging of the life.

Important to mention that the weak interaction is always contains particles and antiparticles, where the neutrinos (antineutrinos) present the opposite side. It means by Feynman's interpretation that these particles present the backward time and probably because this they seem to move faster than the speed of light in the reference frame of the other side.

Finally since the weak interaction is an electric dipole change with ½ spin creating; it is limited by the velocity of the electromagnetic wave, so the neutrino's velocity cannot exceed the velocity of light.

The General Weak Interaction

The Weak Interactions T-asymmetry is in conjunction with the T-asymmetry of the Second Law of Thermodynamics, meaning that locally lowering entropy (on extremely high temperature) causes for example the Hydrogen fusion. The arrow of time by the Second Law of Thermodynamics shows the increasing entropy and decreasing information by the Weak Interaction, changing the temperature dependent diffraction patterns. A good example of this is the neutron decay, creating more particles with less known information about them.
The neutrino oscillation of the Weak Interaction shows that it is a general electric dipole change and it is possible to any other temperature dependent entropy and information changing diffraction pattern of atoms, molecules and even complicated biological living structures.
We can generalize the weak interaction on all of the decaying matter constructions, even on the biological too. This gives the limited lifetime for the biological constructions also by the arrow of time. There should be a new research space of the Quantum Information Science the 'general neutrino oscillation' for the greater then subatomic matter structures as an electric dipole change.
There is also connection between statistical physics and evolutionary biology, since the arrow of time is working in the biological evolution also.
The Fluctuation Theorem says that there is a probability that entropy will flow in a direction opposite to that dictated by the Second Law of Thermodynamics. In this case the Information is growing that is the matter formulas are emerging from the chaos. So the Weak Interaction has two

directions, samples for one direction is the Neutron decay, and Hydrogen fusion is the opposite direction.

Fermions and Bosons

The fermions are the diffraction patterns of the bosons such a way that they are both sides of the same thing.

Van Der Waals force

Named after the Dutch scientist Johannes Diderik van der Waals – who first proposed it in 1873 to explain the behaviour of gases – it is a very weak force that only becomes relevant when atoms and molecules are very close together. Fluctuations in the electronic cloud of an atom mean that it will have an instantaneous dipole moment. This can induce a dipole moment in a nearby atom, the result being an attractive dipole–dipole interaction.

Electromagnetic inertia and mass

Electromagnetic Induction

Since the magnetic induction creates a negative electric field as a result of the changing acceleration, it works as an electromagnetic inertia, causing an electromagnetic mass. [1]

Relativistic change of mass

The increasing mass of the electric charges the result of the increasing inductive electric force acting against the accelerating force. The decreasing mass of the decreasing acceleration is the result of the inductive electric force acting against the decreasing force. This is the relativistic mass change explanation, especially importantly explaining the mass reduction in case of velocity decrease.

The frequency dependence of mass

Since $\boldsymbol{E = hv}$ and $\boldsymbol{E = mc^2}$, $\boldsymbol{m = hv\,/c^2}$ that is the $\boldsymbol{m}$ depends only on the $\boldsymbol{v}$ frequency. It means that the mass of the proton and electron are electromagnetic and the result of the electromagnetic induction, caused by the changing acceleration of the spinning and moving charge! It could be that the $\boldsymbol{m_o}$ inertial mass is the result of the spin, since this is the only accelerating motion of the electric charge. Since the accelerating motion has different frequency for the electron in the atom and the proton, they masses are different, also as the wavelengths on both sides of the diffraction pattern, giving equal intensity of radiation.

Electron – Proton mass rate

The Planck distribution law explains the different frequencies of the proton and electron, giving equal intensity to different lambda wavelengths! Also since the particles are diffraction patterns they have some closeness to each other – can be seen as a gravitational force. [2]

There is an asymmetry between the mass of the electric charges, for example proton and electron, can understood by the asymmetrical Planck Distribution Law. This temperature dependent energy

distribution is asymmetric around the maximum intensity, where the annihilation of matter and antimatter is a high probability event. The asymmetric sides are creating different frequencies of electromagnetic radiations being in the same intensity level and compensating each other. One of these compensating ratios is the electron – proton mass ratio. The lower energy side has no compensating intensity level, it is the dark energy and the corresponding matter is the dark matter.

Gravity from the point of view of quantum physics

The Gravitational force

The gravitational attractive force is basically a magnetic force.

The same electric charges can attract one another by the magnetic force if they are moving parallel in the same direction. Since the electrically neutral matter is composed of negative and positive charges they need 2 photons to mediate this attractive force, one per charges. The Bing Bang caused parallel moving of the matter gives this magnetic force, experienced as gravitational force.

Since graviton is a tensor field, it has spin = 2, could be 2 photons with spin = 1 together.

You can think about photons as virtual electron – positron pairs, obtaining the necessary virtual mass for gravity.

The mass as seen before a result of the diffraction, for example the proton – electron mass rate Mp=1840 Me. In order to move one of these diffraction maximum (electron or proton) we need to intervene into the diffraction pattern with a force appropriate to the intensity of this diffraction maximum, means its intensity or mass.

The Big Bang caused acceleration created radial currents of the matter, and since the matter is composed of negative and positive charges, these currents are creating magnetic field and attracting forces between the parallel moving electric currents. This is the gravitational force experienced by the matter, and also the mass is result of the electromagnetic forces between the charged particles. The positive and negative charged currents attracts each other or by the magnetic forces or by the much stronger electrostatic forces!?

The gravitational force attracting the matter, causing concentration of the matter in a small space and leaving much space with low matter concentration: dark matter and energy.
There is an asymmetry between the mass of the electric charges, for example proton and electron, can understood by the asymmetrical Planck Distribution Law. This temperature dependent energy distribution is asymmetric around the maximum intensity, where the annihilation of matter and antimatter is a high probability event. The asymmetric sides are creating different frequencies of electromagnetic radiations being in the same intensity level and compensating each other. One of these compensating ratios is the electron – proton mass ratio. The lower energy side has no compensating intensity level, it is the dark energy and the corresponding matter is the dark matter.

The Higgs boson

By March 2013, the particle had been proven to behave, interact and decay in many of the expected ways predicted by the Standard Model, and was also tentatively confirmed to have + parity and zero spin, two fundamental criteria of a Higgs boson, making it also the first known scalar particle to be discovered in nature, although a number of other properties were not fully proven and some partial results do not yet precisely match those expected; in some cases data is also still awaited or being analyzed.

Since the Higgs boson is necessary to the W and Z bosons, the dipole change of the Weak interaction and the change in the magnetic effect caused gravitation must be conducted. The Wien law is also important to explain the Weak interaction, since it describes the T_{max} change and the diffraction patterns change. [2]

Higgs mechanism and Quantum Gravity

The magnetic induction creates a negative electric field, causing an electromagnetic inertia. Probably it is the mysterious Higgs field giving mass to the charged particles? We can think about the photon as an electron-positron pair, they have mass. The neutral particles are built from negative and positive charges, for example the neutron, decaying to proton and electron. The wave – particle duality makes sure that the particles are oscillating and creating magnetic induction as an inertial mass, explaining also the relativistic mass change. Higher frequency creates stronger magnetic induction, smaller frequency results lesser magnetic induction. It seems to me that the magnetic induction is the secret of the Higgs field.

In particle physics, the Higgs mechanism is a kind of mass generation mechanism, a process that gives mass to elementary particles. According to this theory, particles gain mass by interacting with the Higgs field that permeates all space. More precisely, the Higgs mechanism endows gauge bosons in a gauge theory with mass through absorption of Nambu–Goldstone bosons arising in spontaneous symmetry breaking.

The simplest implementation of the mechanism adds an extra Higgs field to the gauge theory. The spontaneous symmetry breaking of the underlying local symmetry triggers conversion of components of this Higgs field to Goldstone bosons which interact with (at least some of) the other fields in the theory, so as to produce mass terms for (at least some of) the gauge bosons. This mechanism may also leave behind elementary scalar (spin-0) particles, known as Higgs bosons.

In the Standard Model, the phrase "Higgs mechanism" refers specifically to the generation of masses for the $W^{\pm}$, and Z weak gauge bosons through electroweak symmetry breaking. The Large Hadron Collider at CERN announced results consistent with the Higgs particle on July 4, 2012 but stressed that further testing is needed to confirm the Standard Model.

What is the Spin?

So we know already that the new particle has spin zero or spin two and we could tell which one if we could detect the polarizations of the photons produced. Unfortunately this is difficult and neither ATLAS nor CMS are able to measure polarizations. The only direct and sure way to confirm that the particle is indeed a scalar is to plot the angular distribution of the photons in the rest

frame of the centre of mass. A spin zero particles like the Higgs carries no directional information away from the original collision so the distribution will be even in all directions. This test will be possible when a much larger number of events have been observed. In the mean time we can settle for less certain indirect indicators.

The Graviton

In physics, the graviton is a hypothetical elementary particle that mediates the force of gravitation in the framework of quantum field theory. If it exists, the graviton is expected to be massless (because the gravitational force appears to have unlimited range) and must be a spin-2 boson. The spin follows from the fact that the source of gravitation is the stress-energy tensor, a second-rank tensor (compared to electromagnetism's spin-1 photon, the source of which is the four-current, a first-rank tensor). Additionally, it can be shown that any massless spin-2 field would give rise to a force indistinguishable from gravitation, because a massless spin-2 field must couple to (interact with) the stress-energy tensor in the same way that the gravitational field does. This result suggests that, if a massless spin-2 particle is discovered, it must be the graviton, so that the only experimental verification needed for the graviton may simply be the discovery of a massless spin-2 particle. [3]

The Secret of Quantum Entanglement

The Secret of Quantum Entanglement that the particles are diffraction patterns of the electromagnetic waves and this way their quantum states every time is the result of the quantum state of the intermediate electromagnetic waves. [2] When one of the entangled particles wave function is collapses by measurement, the intermediate photon also collapses and transforms its state to the second entangled particle giving it the continuity of this entanglement. Since the accelerated charges are self-maintaining their potential locally causing their acceleration, it seems that they entanglement is a spooky action at a distance.

Conclusions

The accelerated charges self-maintaining potential shows the locality of the relativity, working on the quantum level also.

The Secret of Quantum Entanglement that the particles are diffraction patterns of the electromagnetic waves and this way their quantum states every time is the result of the quantum state of the intermediate electromagnetic waves.

One of the most important conclusions is that the electric charges are moving in an accelerated way and even if their velocity is constant, they have an intrinsic acceleration anyway, the so called spin, since they need at least an intrinsic acceleration to make possible they movement .

The bridge between the classical and quantum theory is based on this intrinsic acceleration of the spin, explaining also the Heisenberg Uncertainty Principle. The particle – wave duality of the electric charges and the photon makes certain that they are both sides of the same thing. Basing the gravitational force on the accelerating Universe caused magnetic force and the Planck Distribution Law of the electromagnetic waves caused diffraction gives us the basis to build a Unified Theory of the physical interactions.

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