

# Industry Focus



2023 - 2024

## Quantum Chemistry

A curated collection of top articles,  
Thought Leaders and Insights from  
Industry

# TABLE OF CONTENTS

---

**3** ARTICLE  
**What is Quantum Chemistry?**

**7** ARTICLE  
**Applications of Quantum Chemistry**

**11** ARTICLE  
**What is the Time Independent Perturbation Theory?**

**15** ARTICLE  
**The Quantum Mechanical Model of Atoms**

**20** ARTICLE  
**What is the Pauli Exclusion Principle?**

**23** ARTICLE  
**The Quantum Significance of Hydrogen**

**29** ARTICLE  
**Revolutionary Technique Unveils Real-Time Electron Movement in Water**

**34** NEWS  
**Robust Spin-Motion Interaction in the Ultrafast Dynamics of Rydberg Atoms**

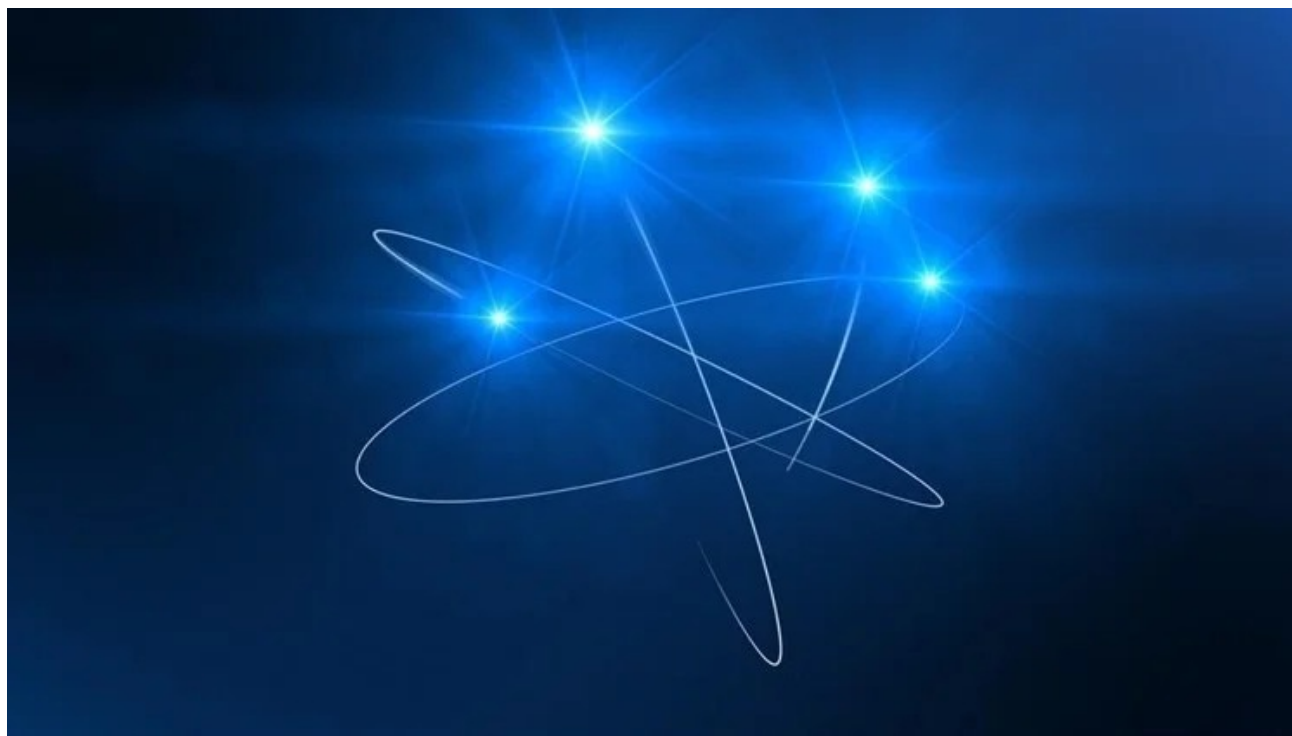


# What is Quantum Chemistry?

By Ilamaran Sivarajah

Apr 18 2022

Quantum chemistry is the application of concepts developed in [quantum mechanics](#) to study the properties of molecules and their reactions.



*Image Credit: alexnako/Shutterstock.com*

Classical mechanics (CM), developed by Isaac Newton, describes the physics of large everyday objects. When the size of the objects becomes much smaller, to microscopic scales, the laws of Newtonian mechanics fail to explain the physics adequately. Quantum mechanics (QM) was formulated in the early 1900s to describe the behavior of matter at the atomic scale. This is critical in chemistry because the scale at which quantum mechanics becomes important is the scale at which electrons, atoms, and molecules exist.

## Differences Between Classical and Quantum Mechanics

Apart from the size of the object studied, there are several properties of QM which differ from CM that are important for understanding chemistry.

QM deals with objects that are very light. For example, fundamental particles of matter like electrons. CM governs the laws of matter that are heavier and macroscopic in nature.

CM is continuous. This means that physical quantities, like position, velocity, energy, or momentum of an object can change in very small amounts. By contrast, in QM, the behavior of objects is discrete or “quantized.” Discrete means there is a finite number of states that a particle can exist in. The energy of a quantum system cannot change its value continuously but can only occupy certain allowed values.

Newton’s equations govern CM. The solutions of Newton’s equations map the trajectory of the object studied. The solutions to the equations are deterministic and can be repeatedly predicted to be the same under the same experimental conditions.

The Schrodinger equation describes the evolution of a quantum system. The equation gives a wave function, which describes the particle as a wave. The wave is spread out over space and it doesn’t have well-defined values for its exact position or momentum. The uncertainties in the position and momentum are described by the Heisenberg Uncertainty Principle. Named after German physicist Werner Heisenberg, the Uncertainty Principle shows that the product of the uncertainty in position and the uncertainty in momentum is greater than or equal to a constant.

Therefore, the solutions to the Schrodinger equation are probabilistic. The wave function gives the probability for various possible outcomes, but it does not give exact outcomes like in a CM trajectory.

Schrödinger's wave equation can be solved exactly for simple quantum systems such as the hydrogen atom. However, for larger atoms and molecules that contain more than one electron, calculating the Schrödinger equation becomes difficult. Solutions are then based on established methods that give approximate results.

## **Molecular Structure**

The internal structure of a molecule is quite complex when compared to atoms. Molecules have internal degrees of freedom like rotational and vibrational states. The addition of extra degrees of freedom makes it difficult to compute structural models of the internal dynamics.

Molecules are linked together by sharing electrons in what is fundamentally known as covalent bonds. Mathematical simulation of covalent bonds takes two prominent approaches. The valence bond model and the molecular orbital model.

## Molecular Bond Theories

The valence bond model describes the creation of a bond orbital, where an electron from two atomic orbitals is shared. The valence bond model, while providing a simple quantum mechanical picture of chemical bonding, does not accurately describe molecules with more than two atoms.

In molecular orbital theory, the electron occupies a molecular orbital that is spread out over the entire molecule. This is different from the valence bond model in that it does not depend on electrons to be localized between two atoms that form a molecular bond. In the molecular orbital theory, summing up the total contributions of each atomic orbital forms the molecular orbital.

Molecular orbital theory calculations produce more accurate results when predicting molecular structure than valence bond theory. Consequently, quantum chemistry simulation software packages rely on molecular orbital methods to calculate molecular structure and dynamics.

## Outlook

Quantum chemical calculations have placed the known elements in the periodic table. Interaction of molecules and atoms with light and their spectroscopic behavior have also been studied in more depth through orbital theories. Further research efforts are undertaken to improve the valence bond and molecular orbital methods for calculating molecular properties.

Experimental data are commonly used to adjust and compare previous calculations to build the models. Computationally challenging quantum chemistry calculations are expected to be solved more efficiently when quantum computers become available.

[More from AZoQuantum: The Quantum Mechanics of Photosynthesis](#)

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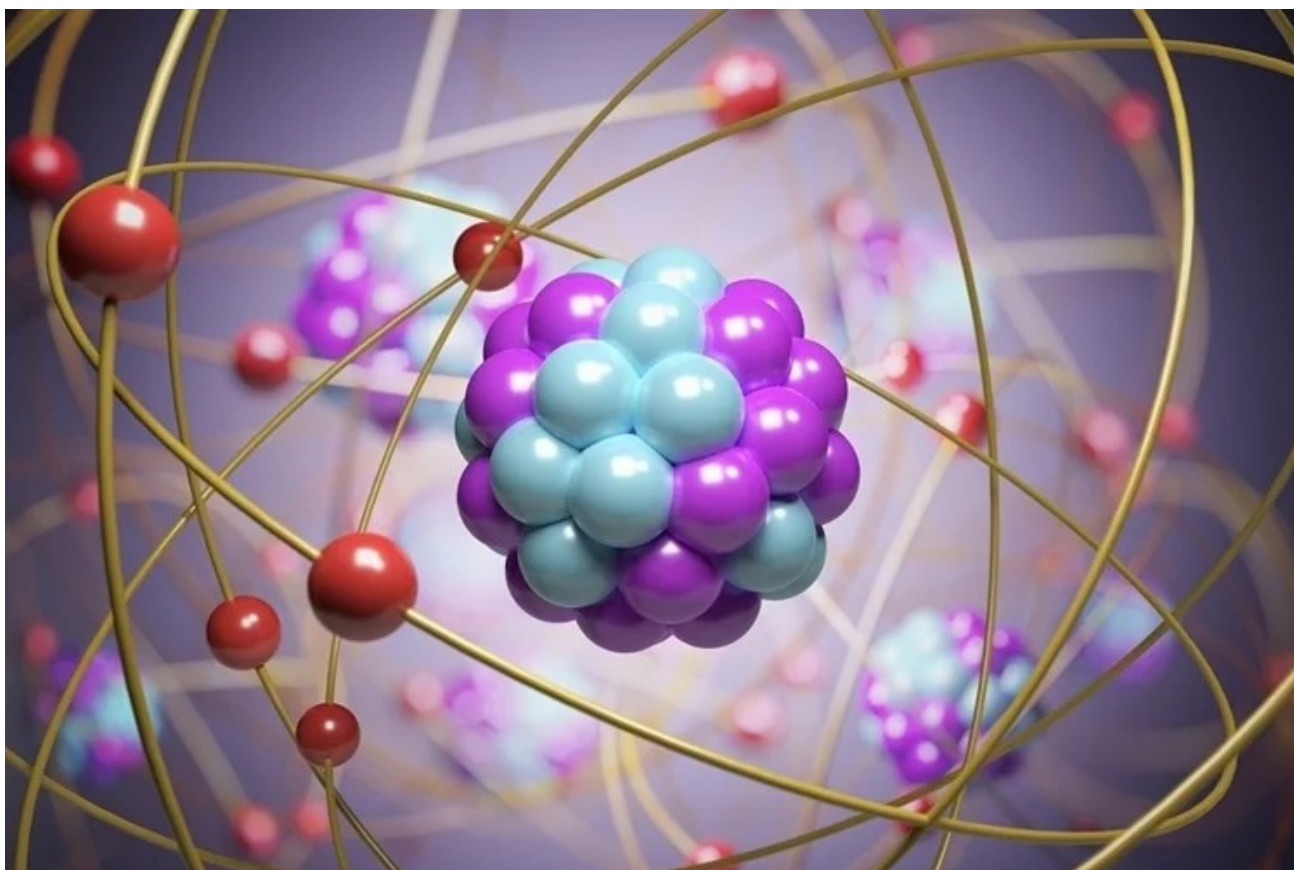
# Applications of Quantum Chemistry



By Kerry Taylor-Smith

Aug 26 2019

Quantum chemistry, also known as molecular **quantum mechanics**, is a division of chemistry that employs quantum mechanics to the study of chemical systems to mathematically describe the fundamental properties of atoms and molecules.



*Image Credits: vchal/shutterstock.com*

At the level of atoms and sub-atomic particles, objects behave very differently to how they might behave normally; quantum theory is an attempt to describe the behavior of matter and energy in this sub-atomic state. Quantum chemistry enables scientists to understand matter at this most fundamental level by using quantum mechanics in physical models and experiments of chemical systems.

Quantum chemistry offers a complete knowledge of the chemical properties of a system and implies the computation of the wave function that describes the electronic structure of

atoms and molecules.

There are two aspects of quantum mechanics which makes quantum chemistry different from previous models of matter;

1. Wave-particle duality – the need to think of very small objects such as electrons as having characteristics of both waves and particles.
2. Quantum mechanical models correctly predict that the energy of atoms and molecules is always quantized, in other words, they only have specific amounts of energy.

Quantum chemistry is a powerful tool to study the ground state of individual atoms and molecules, and the excited and transition states that arise during chemical reactions. Quantum chemical theories allow scientists to explain the structure of the Periodic Table and quantum chemical calculations allow them to accurately predict the structures of molecules and the spectroscopic behavior of atoms. It can be employed to understand, model and forecast molecular properties and their reactions, properties of nanometer materials, and reactions and processes occurring in biological systems.

## Schrödinger and Theoretical Quantum Chemistry

In 1925, Erwin Schrödinger investigated what an electron might look like as a wave-particle around the nucleus of an atom. The result was an equation for particle waves, which now acts as a starting point for the quantum mechanical study of the properties of atoms and molecules.

Theoretical quantum chemistry aims to calculate predictions of quantum theory as atoms and molecules can only have discrete energies. Chemists employ the Schrödinger equation to determine the allowed energy levels of quantum mechanical systems and solving the equation usually the first phase of solving a quantum chemical problem with the result inferring the chemical properties of the material.

However, a precise solution for the Schrödinger equation can only be calculated for hydrogen; because all other atomic, or molecular systems, involve three or more particles, their Schrödinger equations cannot be solved exactly and so estimated solutions are given.



## Quantum Chemistry Methods

There are two commonly used methods to solve Schrödinger's equation – ab initio and semi-empirical methods.

1. Ab initio: A solution to the equation is obtained from the first principles of quantum chemistry using rigorous mathematical approximations and without using empirical methods. It utilizes two strategies to solve the equation: the first is wavefunction based, and the second is density functional-based, which involves the study of the properties of the system through its electronic density, but avoids the explicit resolve of the electronic wavefunction.
2. Semi-empirical methods: these are less accurate and use experimental results to avoid the solution of some terms that appear in ab initio methods.

## Experimental Quantum Chemistry

Experimental quantum chemists rely heavily on spectroscopy – IR spectroscopy, NMR spectroscopy, and scanning probe microscopy – to obtain information about the quantization of energy on a molecular scale. It has great value in supporting and interpreting experimental spectroscopic data. A close collaboration between theoretical calculations and experiments has produced many chances for quantum chemistry calculations to classify species found in spectra and to propose new avenues for experimental study.

## Sources and Further Reading

- [Quantum Chemistry](#)
- [Quantum Chemistry](#)
- [Why is quantum chemistry important?](#)
- [Applications of Quantum Chemistry to Chemical Structure and Reactivity](#)
- [Quantum chemistry](#)
- [Methods and applications in Quantum Chemistry, Life Science and Drug Design software](#)

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# What is the Time Independent Perturbation Theory?

By Ilamaran Sivarajah

Apr 7 2022

The time-independent perturbation theory is a fundamental formalism in [quantum mechanics](#) that describes a quantum system that is affected by a small time-independent external force. This article can be read in tandem with our piece: [What is the Time Dependent Perturbation Theory?](#)

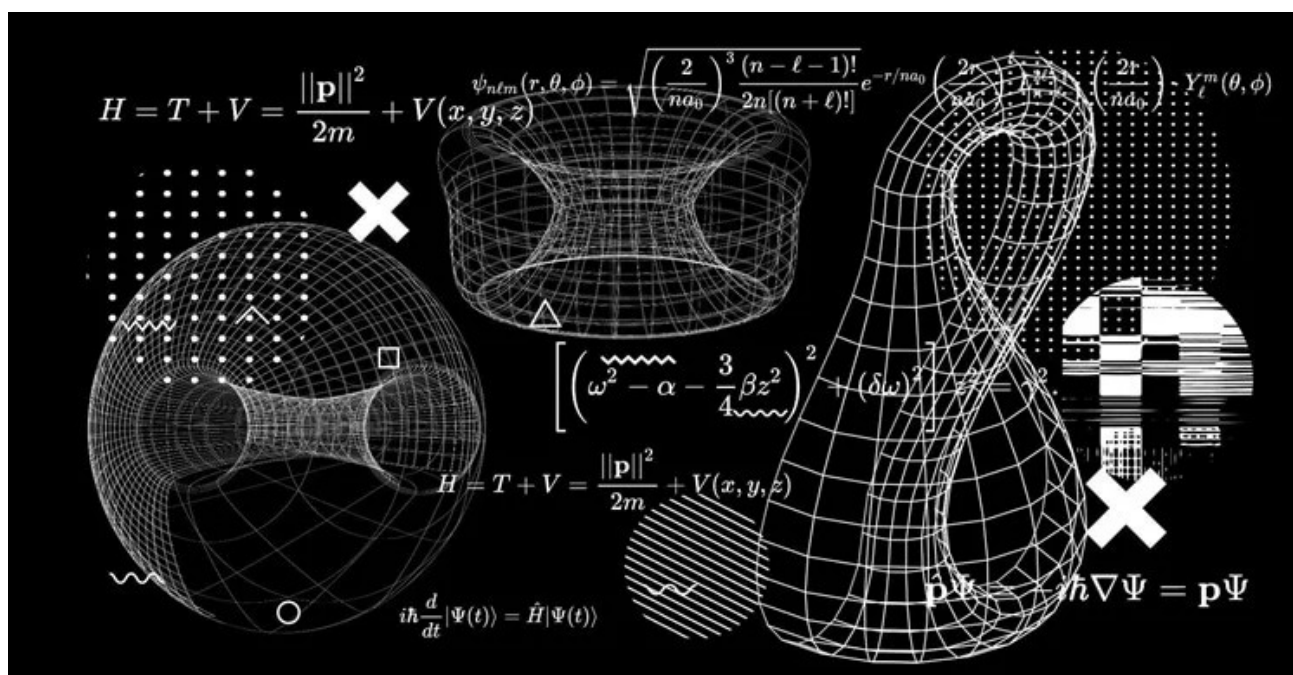


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In nature, a dynamical physical system is described as a set of moving particles. The total energy of such a dynamical system is given by the Hamiltonian.

## The Hamiltonian

The Hamiltonian is a mathematical definition formulated by Sir William Rowan Hamilton in 1835

The Hamiltonian of a physical system is its total energy given by the sum of the kinetic energy and the potential energy. The Hamiltonian of a classical physical system can be represented as shown in the equation below.

$$H = K + V$$

Where  $H$  denotes the Hamiltonian, which is the sum of kinetic energy  $K$  and potential energy  $V$ .

In quantum mechanics, the Hamiltonian of the system is represented by quantum mechanical operators. The kinetic and potential energy expressions are transformed to their associated operator representations as shown below.

$$\hat{H} = \hat{K} + \hat{V}$$

## The Schrodinger Equation

The Schrodinger equation, which is a significant landmark in the development of quantum mechanics, is derived when the Hamiltonian is applied to the energy wave function. A wave function is a mathematical description of the quantum state of an isolated quantum system.

In the time-independent Schrodinger equation, the operation produces specific values for the energy called energy eigenvalues. A measurement of an arbitrary dynamic physical system's total energy using the Hamiltonian provides a set of possible solutions.

The harmonic oscillator, the infinite square well, and the hydrogen atom are some examples of problems that can be solved using the Hamiltonian operation and the Schrodinger equation.

## Time Independent Perturbation Theory

To understand perturbation theory, it is ideal to analyze a problem that can already be solved using the Schrodinger equation. For example, the hydrogen atom. A perturbation is a small change that is introduced to the system. This change can be an electric or magnetic field or any other subtle force. In the time-independent case, the perturbing force is uniform and does not vary with time.

The small change introduces a perturbation to the total energy of the system or the Hamiltonian of the system. This perturbation distorts the original Hamiltonian. This subtle change can be represented by a new Hamiltonian in the following way;



$$\hat{H} = H^0 + H_1$$

((hereby referred to in the text as  $H^0$ ,  $H_0$ , and  $H_1$ , respectively))

where  $H^0$  is the new Hamiltonian,  $H_0$  is the original Hamiltonian that can be solved, and  $H_1$  is the perturbation that has been introduced.

To solve the new Hamiltonian, the quantum states have to be expanded. The quantum states of the perturbed Hamiltonian can be expanded as superpositions of the known solutions of the unperturbed Hamiltonian. The perturbation can be thought of as the change in solution states from the original states to a new perturbed state. The perturbed states are the original states plus some additional elements that have been introduced by the external force.

The solutions to the original Hamiltonian are used as the basis to describe the solutions to the perturbed Hamiltonian. The energy of the perturbed state is analyzed with a series expansion like the power series or Taylor series. The zeroth term of the series expansion is the unperturbed energy and the other terms represent the first-order correction and the second-order correction and so on. In many cases, considering just the first few terms of the power series give reasonable results. Adding the appropriate correction results in an approximate solution for the perturbed Hamiltonian.

## Examples of Time Independent Perturbation Theory

Two examples where time-independent perturbation theory predicts approximate solutions are the Zeeman effect and the Stark effect.

When a homogeneous magnetic field is introduced to a system that has a magnetic dipole moment, like the hydrogen atom, the energy levels are split into sublevels. This effect is called the Zeeman effect. Similarly, the Stark effect is the electric analog to the Zeeman effect. An atom carrying an electric dipole moment, like the hydrogen atom, will get a splitting of its energy levels when an exterior homogeneous electric field is turned on.

While the time-independent perturbation theory is a key fundamental concept widely used

in quantum mechanics, it has limitations when computing many-body systems. Many-particle systems present various contributions to the physical nature of the problem that makes the computations impossible to handle. Even in the case of the hydrogen atom, the external field has to be small compared with the electric field inside the atom for the approximation to be accurate.

### What is the Time Dependent Perturbation Theory?

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# The Quantum Mechanical Model of Atoms



By Owaiss Ali

Oct 27 2023

From the classical models of the 18th century to the quantum revolution of the 20th century, our understanding of atomic structure has evolved. With its probabilistic nature, the quantum mechanical model has fundamentally reshaped our perception of atoms. This article explores the origins and fundamentals of this groundbreaking model.



*Image Credit: Marko Aliaksandr/Shutterstock.com*

## Historical Development of Atomic Models

The quest to comprehend atomic structure began in earnest in the early 1800s. British scientist John Dalton proposed an early atomic theory, picturing atoms as tiny, solid, indivisible spheres. This was followed in the late 19th century by J.J. Thomson's "plum pudding" model, which depicted the atom as a diffuse cloud of positive charge with electrons embedded throughout like plums in a pudding.

However, a key experimental result in 1909 upended established conceptions of atomic structure. Physicist Ernest Rutherford directed alpha particles at a thin gold foil and detected that a small fraction rebounded backward. This suggested that the positive charge and nearly all the mass of an atom is concentrated in a tiny, dense nucleus, contrary to the plum pudding model.

Rutherford conceived the atom as a compact central nucleus orbited by electrons at a distance, akin to planets revolving around the sun. However, this raised a problem: according to classical electromagnetism, the orbiting electrons should continuously lose energy and fall into the nucleus.

Around this time, the discovery of quantized energy levels and emission spectra pointed to deficiencies in classical physics when applied at atomic scales. To address this, physicist Niels Bohr integrated the newly proposed quantum concepts into Rutherford's model. He postulated that electrons occupied discrete circular orbits at set distances from the nucleus, jumping between fixed energy levels and emitting photons when changing orbits.

While Bohr's model successfully explained patterns in atomic spectra and the stability of matter, issues remained. It relied heavily on classical notions of definite electron orbits that did not fit with emerging quantum theory. The model also could not explain finer details of atomic spectra and failed to account for electron properties like spin and magnetic moment.

As a result, the stage was set for a new model of atomic structure based firmly on the principles of [quantum mechanics](#).

## The Schrödinger Equation and Quantum Mechanical Model of Atoms

In contrast to Niels Bohr's conception of electrons as discrete particles orbiting the atomic nucleus in fixed paths, Erwin Schrödinger, inspired by de Broglie's particle-wave duality, postulated that the behavior of electrons could be mathematically described as matter waves. This model, known as the quantum mechanical model, laid the foundation for modern understanding of the atomic structure.

The quantum model describes the electrons probabilistically, using Schrodinger's wave equation to determine the likelihood of finding an electron at any given location.



$$\hat{H}\psi = E\psi \text{ (Basic form of Schrödinger Equation)}$$

Here,  $\hat{H}$  represents the Hamiltonian operator, which defines the total energy of a quantum particle, and  $E$  is the particle's actual total energy. The wave function  $\psi$  at a point in space represents the electron's matter wave amplitude, though it often contains complex values.

However, the square of the magnitude of a wavefunction,  $|\psi|^2$ , is significant as it describes the probability of finding an electron within a specific region, serving as the probability density. Schrödinger identified these regions of space as electron orbitals, which differ from Bohr's circular orbit/planetary model.

In Schrödinger's quantum model, electrons are more accurately described as existing in "clouds" around the nucleus, organized into shells or orbitals at varying distances. The Schrödinger equation solutions (quantum numbers) provide the energetics and spatial distribution of electrons in orbitals.

Similar to Bohr's model, the energy of an electron in an atom is quantized with specific allowable values. The key distinction between Bohr's model and Schrödinger's approach is that Bohr introduced quantization arbitrarily, whereas in Schrödinger's approach, quantization naturally arises from the wave equation.

This quantum model effectively addressed inconsistencies in the classical Rutherford-Bohr theory and offered improved agreement with spectroscopic experiments. The quantum mechanical framework also provided a natural explanation for the intrinsic properties of electrons, including spin and magnetic moment, which arise from the underlying wave-particle duality.

## Quantum Numbers and Atomic Orbitals

The quantum mechanical model uses four quantum numbers to define the atomic orbitals and their electron distribution.

1. **Principal Quantum Number ( $n$ ):** Describes an electron's energy level and average distance from the nucleus. It takes positive integer values (1, 2, 3, etc.), with higher values indicating higher energy levels.

2. **Angular Momentum Quantum Number ( $l$ ):** Determines the shape of the orbital, whether it is a spherical s-orbital, dumbbell-shaped p-orbital, clover-shaped d-orbital, and so on
3. **Magnetic Quantum Number ( $m_l$ ):** Indicates the spatial orientation of orbitals and varies from  $-l$  to 0 to  $+l$  based on the value of  $l$ .
4. **Spin Quantum Number ( $m_s$ ):** Describes an electron's spin in a magnetic field as either  $+1/2$  (clockwise) or  $-1/2$  (counterclockwise), with each subshell accommodating two electrons with opposite spin values.

## Electron Spin and Pauli Exclusion Principle

Austrian physicist Wolfgang Pauli established a fundamental principle, the Pauli exclusion principle, which provides the final information needed to comprehend the overall behavior of electrons within atoms.

This principle is based on the electron spin quantum number, representing the electron's intrinsic spinning motion. It restricts how electrons can be configured within an atom, stating that no two electrons in the same atom can possess an identical set of all four quantum numbers. Therefore, each orbital can contain a maximum of two electrons with opposite spin quantum numbers  $+1/2$  and  $-1/2$ .

## Concluding Remarks

Despite its complexities, the quantum mechanical model excelled in explaining observations, notably in the hydrogen spectrum, where quantized orbital energies derived from quantum numbers produced multiple spectral lines. This model extended to multi-electron atoms, departing from classical particle-based views to embrace probabilities, wavefunctions, quantized energies, spin, and quantum numbers as fundamental attributes governing particles' behavior, shaping atomic and molecular structure. This transformation is a remarkable achievement in humanity's quest to understand the atom, serving as the foundation of chemistry and materials science.

[New Particles and Physics Beyond the Higgs Boson](#)

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# What is the Pauli Exclusion Principle?



By Bismay Prakash Rout

Dec 31 2021

This article provides an overview of the Pauli Exclusion Principle and its enduring relevance.

# PAULI

*Image Credit: idesignf/Shutterstock.com*

In January 1925, Austrian physicist Wolfgang Pauli, after empirically analyzing the electron emission spectrum, proposed that each electron in an atom has a different combination of quantum numbers than any other electron present in the same atom. This is known as the Pauli exclusion principle. This theory is true for electrons and half-integer spinning fermions and their combinations such as quarks, protons, and neutrons but not valid for integer spinning bosons such as photons produced by a laser or atoms in a Bose-Einstein condensate.

The meaning of half-integer spin is that the intrinsic angular momentum of each fermion is a half-integer ( $1/2, 3/2, 5/2, \dots$ ) multiple of reduced Planck constant ( $\hbar = h/2\pi$ ). Moreover, other than fermions, many atoms such as helium-4 or nuclei such as sodium-23 nucleus also obey the exclusion principle owing to the asymmetric half-integer spinning.

The exclusion principle is also the base of the accepted [quantum mechanics](#) theory that everything in the universe has a discrete or combination of discrete energies state, which is



contrary to the continuity assumption in classical mechanics. There are four quantum numbers viz. principal quantum number ( $n$ ), azimuthal quantum number ( $l$ ), magnetic quantum number ( $m_l$ ), and spin quantum number ( $m_s$ ) that describes the specific state of an electron in an atom such as energy level, distance from the nucleus, number of sub-shell, the shape of orbitals, and spin orientation.

## Ramifications of Pauli Exclusion Principle

Based on the nuclear shell model, an atom of an element in a stable state has a fixed number of protons and an equal number of electrons, also known as the atomic number, and each electron has a specific quantum number set, this is the fundamental basis of arrangement of each element in the modern periodic table.

Furthermore, this principle helps explain certain astrophysical phenomena such as the stability and collapsing of stars. As we know, stars have enormous mass, which produces a massive gravitational pull to gas particles towards their core, but it is counterbalanced by the pressure generated during the fusion process; thus, only a few stars of certain minimum mass survive the formation process.

[More from AZoQuantum - Frontera: An Overview of the World's Fastest Academic Supercomputer](#)

Subsequently, when the internal temperature of a star approximately surpasses a hundred million Kelvin, its core fails to sustain the fusion process and they become red giants followed by a catastrophic collapse under massive gravitational pull.

For small and medium-sized stars this collapse is halted to a certain degree by the opposing electron degeneracy pressure and neutron degeneracy pressure. As explained by the Paul exclusion principle, each fermion has a specific quantum state and they repulse each other during compression, resulting in the generation of opposing force.

If the mass of the star is below 1.4 times the solar mass, the electron degeneracy pressure dominates, and a white dwarf is formed, whereas if the mass of the star is between 1.4 – 3 times the solar mass, the neutron degeneracy pressure leads, and a neutron star is formed. However, both degeneracy pressures fail when the mass of the star is too high, resulting in the formation of a black hole.

Although the Pauli exclusion principle gives the idea of the unique state of each electron or fermion in an atom, it can not explain the uncertainty principle in quantum mechanics, which states that it is not possible to assign exact instantaneous value to the position and momentum of an electron in an atom.

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[Pauli Exclusion Principle: What Is It & Why Is It Important? \(sciencing.com\)](http://sciencing.com)

[Pauli Exclusion Principle \(gsu.edu\)](http://gsu.edu)

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# The Quantum Significance of Hydrogen



By Robert Lea

Oct 19 2021

Hydrogen may be the Universe's most common and simplest element, but it is important not to underestimate its importance to the physics of the very large and the infinitesimally small.



*Image Credit: Corona Borealis Studio/Shutterstock.com*

New research suggests a new model for hydrogen-based upon a fusion of quantum physics and computational science.

This fascination with hydrogen for science isn't new, and it's hardly surprising as this element is woven through all of physics, just as it threads through the fabric of the Universe itself.

One proton, orbited by one electron. That's hydrogen in its most basic form. The Universe's most common element. Atomic number 1. Sat at the top of the periodic table.

Non-scientists may initially struggle to understand why physicists get so excited about hydrogen. But, any astronomer will quickly correct this.

## Stars and Simplicity

For life here on Earth, energy from the sun is everything, and the sun could not produce energy if not for hydrogen.

Every star during its lifetime, which astronomers call the main sequence, is burning hydrogen in its core; the sun is essentially a giant burning ball of hydrogen and some helium.

When the hydrogen in the center of our star is exhausted in around 5 billion years, it will no longer be able to protect itself against gravitational collapse. As its core falls in on itself, the energy released will cause the sun's outer layers to expand.

This expansion will reach out to the orbit of Mars, meaning the sun, now a red giant star, will consume the inner rocky worlds of the solar system, including Earth.

By the time the pressure in the core is enough to facilitate the burning of helium into heavier elements like carbon, Earth and her sister worlds, Mercury, Venus, and Mars, will be destroyed.

This means that hydrogen in the sun is almost analogous to sand in a cosmic hourglass; when it's gone, our time is up.

## Hydrogen in the Early Universe

In the earliest moments of the Universe, mere picoseconds after that initial burst of expansion that we call the Big Bang, the Universe was too hot and dense for any element to exist.

At around 0.000006 seconds the first particles, neutrinos, quarks, and electrons formed. After around three minutes the Universe had cooled enough to reach  $10^9\text{K}$ .

This is known as the era of nucleosynthesis, when the first hydrogen atoms formed, followed by helium atoms. The proportions of these elements in the early Universe were hydrogen at 75 percent, helium at 25 percent, with just a trace of heavier elements; mostly lithium.



## [More About Our Universe: Direct Detection fo Dark Energy - An Interview With Dr. Sunny Vagnozzi](#)

One of the most impressive aspects of our theory of the Big Bang is the fact that it has been able to precisely predict the relative abundances of these early elements.

These primordial elements went on to form the first generation of stars, which would in turn play host to the nuclear processes that would go on to create the remaining elements forming the rest of the periodic table.

Hydrogen is not just vital at these tremendous cosmic scales, however. It is also pretty important when considering theories of the very small.

## Hydrogen as a Simple Quantum Mechanical Model

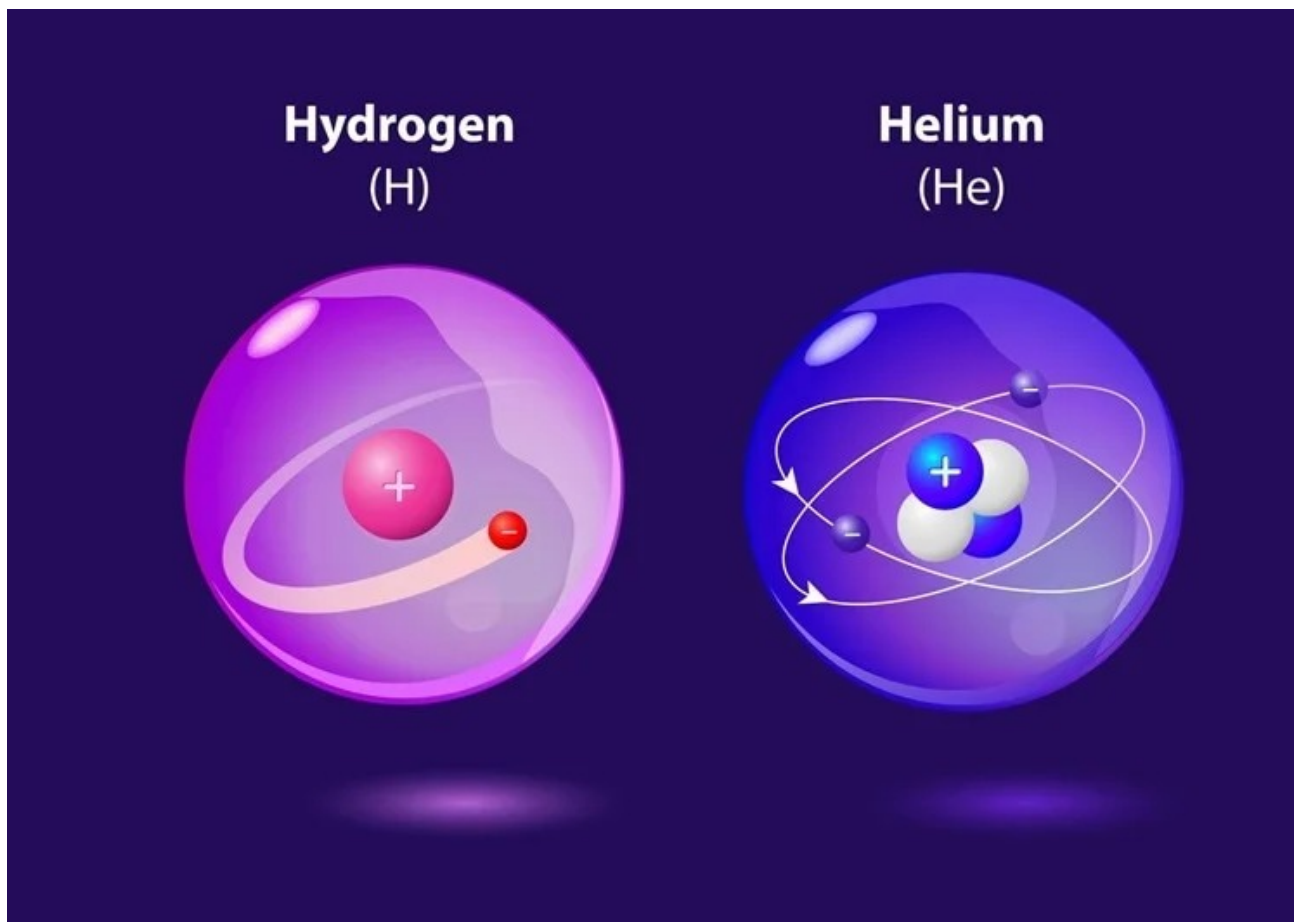
The idea of quantum physics being simple is probably anathema to most physicists and non-physicists alike. However, hydrogen and its relatively simple composition are vital to helping demonstrate the rules of quantum physics.

The name “quantum” comes from the Latin word “quanta” meaning “how much”, which was adopted by Max Planck when he was first developing the earliest theories of [quantum mechanics](#).

Albert Einstein had previously discovered something called the photoelectric effect, a phenomenon in which light hits metal and causes the release of electrons. The theory would earn Einstein the Nobel in 1921, and is probably commonly encountered by most people when they walk through an automatic door; the opening mechanism of most of these doors is built upon the photoelectric effect.

Here emerges the part of the photoelectric effect that leads to the discuss of quantum physics and hydrogen. What Einstein found was that the intensity of light, the number of photons, shone on a strip of metal, did not influence the release of electrons.

You could shine long-wavelength, low-frequency light on a sheet of metal all day and it would not release a single electron. Switch that out for a high-frequency, short-wavelength light and in seconds electrons would be flying everywhere.



*Image Credit: Designua/Shutterstock.com*

The reason for this is that photons come as “packets” of energy that could take certain values intrinsically tied to frequency and wavelength. Only one of these packets or “quanta” with enough energy can shake loose an electron.

The best way of considering this is looking at what happens to electrons around atoms. Because multiple electrons can have a screening effect that makes the situation more complicated, the easiest way to do this is by looking at an element that consists of one electron around one proton: hydrogen.

An electron around a proton has a ground state energy of -54.4 electron volts (eV); to liberate that electron—to set it completely free from the proton—you have to get it to absorb a photon of 54.4 eV or more.

Two photons of 27.2 eV will not be enough, nor will photons of 53 eV or 1.4 eV. Only a photon with 54.4 eV or more will liberate that electron.

However, ground state and completely free are

not the only energy states for electrons. When around an atomic nucleus, an electron can go through several excited states or electron shells.

For hydrogen, the first excited state can be occupied by an electron with -13.6 eV, the second -6.04 eV, and so on.

So, if one imagines an electron at the ground state in a hydrogen atom absorbing a photon of 40.8 eV, it will “step up” to that first excited state. It won’t stay excited for too long; eventually—and unpredictably—it will emit a photon of 40.8 eV and drop back down to the ground state.

An analogy is that electrons in an atom are like a ladder. Your foot can rest at any rung for a time, just like an electron can sit at any energy state. But, neither your foot nor the electron can rest between rungs or energy levels respectively.

## A Hydrogen Thread Linking Science’s Future to Its Past

The dawn of quantum mechanics was at the start of the 20th century, but it is the importance and applicability of hydrogen that is still inspiring research today. Recently it inspired Jeevake Attapatu’s paper, which also acts as this doctoral thesis.

Attapattue takes a thoroughly modern approach to modeling the behavior of hydrogen, using machine learning to understand its conductive properties and its temperature.

Using methods that wouldn’t be available to their peers, modern scientists are still unpicking the mysteries of this allegedly simple element, creating a thread from the future to the past of science.

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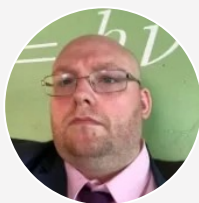
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# Revolutionary Technique Unveils Real-Time Electron Movement in Water



By Owais Ali

*Reviewed by Lexie Corner*

Mar 5 2024

In a recent study published in *Science*, researchers have directly observed the real-time motion of electrons in water using intense X-Ray laser pulses. They achieved this by isolating the electronic response with precisely timed attosecond pulses, preventing molecular framework movement during experimentation.



*Image Credit: Siwakorn1933/Shutterstock.com*

Monitoring the rapid movement of electrons in molecular systems following ionization or excitation has been a key objective in chemistry and physics. However, tracking ultrafast electron dynamics on the attosecond timescale ( $10^{-18}$  seconds) poses a significant challenge, as conventional laser-based spectroscopy is limited to femtosecond ( $10^{-15}$  s) resolution.

The X-Ray attosecond transient absorption spectroscopy (AX-ATAS), operating on the attosecond timescale, overcomes this limitation and enables the separation of electronic responses from slower nuclear motions that previously obscured observation.

*"We now have a tool where, in principle, you can follow the movement of electrons and see newly ionized molecules as they're formed in real-time,"* says Linda Young, Senior author of the study and Distinguished Fellow at the U.S. Department of Energy's Argonne National Laboratory.

## All-X-Ray Attosecond Pump-Probe Spectroscopy

The researchers conducted these experiments at the [Linac Coherent Light Source](#) (LCLS) in the SLAC National Accelerator Laboratory.

LCLS generates extremely short (approximately 10-100 attosecond), intense X-Ray free electron laser (XFEL) pulses via acceleration of electron bunches to high energy, followed by rapid deceleration upon injection into arrays of alternating magnets called undulators. This forces the electrons to emit synchronized X-Ray photons that can be focused down to micron spots on a sample.

One significant innovation was the generation of precisely timed pairs of attosecond X-Ray pulses using a specialized double undulator configuration at LCLS. This enabled the researchers to implement an "all X-Ray" attosecond pump-probe spectroscopy scheme.

In this setup, the first pump pulse ionized a liquid water sample, while the second probe pulse measured the induced electronic structural changes 700 attoseconds later, minimizing distortion from nuclear dynamics. This configuration overcomes limitations associated with coupling ultrafast optical and X-Ray pulses for attosecond spectroscopy.

With advanced jet technology to flow a thin sheet of pure liquid water across the approximately 10  $\mu\text{m}$  diameter XFEL beam focus, the stage was set to visualize electron processes in an aqueous system faster than ever.

## Real-Time Tracking of High-Energy Electron States in Water

When the intense XFEL pump pulse removes (ionizes) a core 1s electron from a water molecule, the created hole can be filled rapidly by electrons descending from the outer valence orbitals on a sub-femtosecond timescale.



This electronic relaxation initiates a characteristic sequence of transient intermediate states with holes (unoccupied orbitals) in various valence locations. By tuning the XFEL probe pulse energy to core-level absorptions sensitive to these valence vacancies, the researchers could visually track the hole migration among valence states populated within the first few hundred attoseconds following the ionization of water.

The researchers also observed that the distinct double-peak feature of the  $1b_1$  absorption signal (fingerprinting population of  $1b_1$  valence holes), which vanishes within approximately 700 attoseconds after ionization, does not reflect two distinct structural motifs of liquid water at equilibrium—contrary to previous interpretations.

Instead, their findings demonstrate that this transient spectral signature arises from ultrafast distortion of the  $1b_1$  orbital itself, induced by sub-femtosecond electron dynamics initiated by ionization.

## Reshaping Our Understanding of Water Structure

This discovery has far-reaching implications as it resolves a decade-long controversy regarding the origin of the split  $1b_1$  peak universally observed in X-Ray measurements of liquid water. Previously, the distinct low and high-energy components of this signal were alternatively interpreted as evidence for two different hydrogen-bonded structural motifs intrinsically existing in ambient water, in contrast to simpler models picturing a homogeneous network of molecules.

However, hydrogen atom motions occur on similar timescales of a few hundred femtoseconds, which could also cause the split peak shape without requiring distinct structural species. Previous experiments could not distinguish between these pictures.

The sub-femtosecond temporal resolution achievable with AX-ATAS allowed the researchers to unambiguously demonstrate that the dual  $1b_1$  component arises from ultrafast dynamical distortion rather than intrinsically heterogeneous structural motifs. This represents a significant advancement in the field.

*"Basically, what people were seeing in previous experiments was the blur caused by moving hydrogen atoms. We were able to eliminate that movement by doing all of our recording before the atoms had time to move,"* says Linda Young.

By exploiting the unprecedented capability of XFELs to outpace nuclear motion, this work

illustrates how tracking purely electronic phenomena can paradoxically provide new insights into the arrangement of atoms at equilibrium.

## Conclusion

The study establishes AX-ATAS as a groundbreaking technique for researching high-energy quantum states and electron dynamics activated by ionizing radiation. Initially tested on liquid water, the method holds potential for application in diverse systems, broadening insights into attosecond-scale electronic dynamics.

*"The methodology we developed permits the study of the origin and evolution of reactive species produced by radiation-induced processes, such as encountered in space travel, cancer treatments, nuclear reactors, and legacy waste,"* explains Linda Young.

Ongoing AX-ATAS developments will broaden its application to diverse materials, enhancing precision and efficiency to reveal fundamental principles of electron dynamics and correlation during chemical transformations on an attosecond scale in complex systems.

**[More from AZoQuantum: How do Hydrodynamic Electrons Flow in 3D Materials?](#)**

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**Written by**

**Owais Ali**

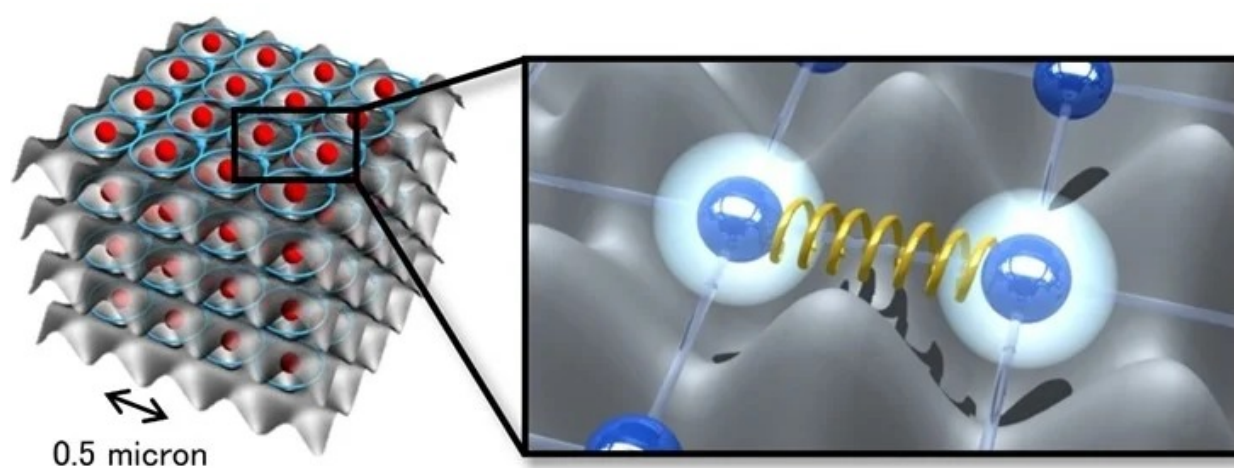
NEBOSH certified Mechanical Engineer with 3 years of experience as a technical writer and editor. Owais is interested in occupational health and safety, computer hardware, industrial and mobile robotics. During his academic career, Owais worked on several research projects regarding mobile robots, notably the Autonomous Fire Fighting Mobile Robot. The designed mobile robot could navigate, detect and extinguish fire autonomously. Arduino Uno was used as the microcontroller to control the flame sensors' input and output of the flame extinguisher. Apart from his professional life, Owais is an avid book reader and a huge computer technology enthusiast and likes to keep himself updated regarding developments in the computer industry.

# Robust Spin-Motion Interaction in the Ultrafast Dynamics of Rydberg Atoms

Reviewed by Danielle Ellis, B.Sc.

Sep 4 2024

According to a study published in *Physical Review Letters* on August 30<sup>th</sup>, 2024, researchers at the Institute for Molecular Science discovered quantum entanglement between electronic and motional states in their ultrafast quantum simulator, which is caused by the repulsive force caused by the strong interaction between Rydberg atoms.



*Atoms in the optical lattice, trapped at a distance of 0.5 micron, are excited to the Rydberg state by the ultrafast excitation technique. Interaction between close Rydberg atoms results in the repulsive force. Image Credit: Takafumi Tomita (Kenji Ohmori group)*

They also suggest a novel quantum simulation approach that incorporates repulsive forces between particles.

Cold atoms trapped and constructed by optical traps have gained interest as a platform for quantum technology applications such as quantum computing, modeling, and sensing. Quantum entanglement, or the correlation between quantum states of corresponding atoms, is fundamental in quantum technology. Rydberg states, or giant electronic orbitals, are utilized to produce quantum entanglement on cold atom platforms.

The authors of this study thoroughly investigated the quantum state in the ultrafast quantum simulator, and they discovered that the quantum entanglement between electronic and motional states is created by the powerful repulsive force between atoms in the Rydberg

state, along with the quantum entanglement between atoms' electronic states.

After being cooled to 100 nanokelvin via laser cooling, the 300,000 Rubidium atoms were placed into the optical trap to form an optical lattice with a 0.5 micron spacing.

Subsequently, an ultrashort pulse laser light lasting just 10 picoseconds was used to produce the quantum superposition of the ground state with an electron in the 5s orbital and the Rydberg state with an electron in the gigantic 29s orbital.

Previous studies limited the distance between Rydberg atoms to around 5 microns because a Rydberg atom prevents adjacent atoms from being excited to the Rydberg state, a phenomenon known as Rydberg blockade. The scientists avoided this effect by using ultrafast stimulation with an ultrashort pulse laser light.

Observing the time development of the quantum superposition, the scientists discovered that quantum entanglement between electronic and motional states and entanglement among electronic states form in a few nanoseconds.

This can be explained by the repulsive force between atoms in the Rydberg state caused by the extremely strong interaction, which introduces the connection between “either the atom is in the Rydberg state or not” and “either the atom is moving or not.”

This phenomenon arises only when Rydberg atoms are close to the spread of the atomic wavefunction in the optical lattice (60 nanometers). The scientists' unique ultrafast excitation approach, which allows for a distance of 0.5 microns, made its detection possible.

The researchers also presented a novel quantum simulation approach that incorporates repulsive forces between particles, such as electrons in materials. The repulsive force may be introduced by stimulating atoms in Rydberg states on a nanosecond scale with ultrafast pulse lasers.

By doing this repeatedly, the repulsive force between atoms trapped in the optical lattice can be arbitrarily regulated. This approach is anticipated to provide a novel quantum simulation using the motional states of particles with repulsive forces.

This study's research group is also gaining attention for constructing an ultrafast cold-atom quantum computer that speeds up a two-qubit gate operation by two orders of magnitude compared to traditional cold-atom quantum computers.

The ultrafast cold-atom quantum computer uses Rydberg states to accomplish a two-qubit gate operation, and the influence of atomic motion during the interaction is one of the primary reasons for the operation's fidelity to be reduced.

The study empirically disclosed the method by which quantum entanglement between electronic and motional states is formed, which represents significant progress in improving the fidelity of the two-qubit gate operation and creating socially usable quantum computers in the future.

## Journal Reference:

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