Quantum Chaos: Bridging Quantum Mechanics and Classical Chaos

PHYD38 Nonlinear Systems and Chaos

Ivan Pakhomov, Ethan Harris, Haoyan Zeng

March 2024

1 Introduction

Classical mechanics, as elucidated by Newton, provides a framework in which the motion of objects is governed by precise differential equations. A dynamical system consists of a set of states Ω and an evolution law that dictates how these states propagate in time, whether discretely or continuously. The set Ω encompasses all possible states, describing the physical reality being modelled and referred to as the phase space. The evolution law is time-independent. In this model, given the initial conditions, the motion of the system is entirely predictable, which is suitable for simple models that yield analytical solutions.

However, in reality, most systems of equations lack simple analytical solutions, necessitating the use of numerical methods for accurate predictions, even though the system's evolution is deterministic. In the late 19th century, Henri Poincaré first recognized this sensitivity to initial conditions in classical systems, laying the foundation for understanding chaotic behaviour. A chaotic system may have sequences of values for the evolving variable that exactly repeat themselves, giving periodic behaviour starting from any point in that sequence. However, such periodic sequences are repelling rather than attracting, meaning that if the evolving variable is outside the sequence, however close, it will not enter the sequence and, in fact, will diverge from it. Thus, for almost all initial conditions, the variable evolves chaotically with non-periodic behaviour. Additionally, chaotic motion must be non-integrable to exhibit chaotic phenomena. "Butterfly effect," a term coined by Edward Lorenz, exemplified this unpredictability. In 1961, Lorenz discovered that minute differences in initial conditions, such as starting his simulation from a rounded-off value, led to vastly different outcomes, highlighting the sensitivity of chaotic systems to initial conditions.

Chaos theory challenges the notion of perfect predictability in classical systems. While these systems are deterministic in principle, their behaviour can be highly unpredictable, emphasizing the importance of understanding and accounting for chaos in complex systems analysis. Chaotic motion is transitive, meaning the trajectory nearly visits every point in the phase space as time progresses. Additionally, chaotic motion must be non-integrable to exhibit chaotic phenomena.

The study of chaos is crucial in various fields, from meteorology to economics, where small perturbations can have significant impacts on outcomes. Applications of chaos theory extend beyond physics and mathematics into various other fields, including biology and economics. In biology, chaotic behaviour has been observed in population dynamics, ecological systems, and the behaviour of neurons in the brain. Chaotic models have been used to study complex phenomena such as the dynamics of predator-prey relationships, population growth, and the spread of diseases. In economics, chaos theory has been applied to understand the behaviour of financial markets, where seemingly random fluctuations can exhibit underlying patterns of chaos. Models based on chaos theory have been used to study stock market dynamics, the impact of policy changes on economic systems, and the behaviour of complex economic networks.

These applications demonstrate the broad relevance and impact of chaos theory across diverse fields, highlighting its utility in understanding and predicting complex, nonlinear systems.

After some exploration of chaos on a macro scale, the question arose: How would atomic systems behave if classical systems were chaotic? According to Bohr's correspondence principle, quantum systems governed by quantum mechanics should correspond to classical behaviour when quantum numbers are very large. This suggests that some vestiges of classical chaos should persist in quantum mechanics.

However, the linear nature of the Schrödinger equation, the governing principle of quantum mechanics, seemingly contradicts the existence of chaos in quantum mechanics. Furthermore, under the uncertainty principle, infinitesimal changes in initial conditions are unattainable in the quantum world, further complicating the notion of chaos in quantum mechanics.

Exciting experiments have been conducted on highly excited Rydberg atoms in strong magnetic fields, where their classical descriptions become chaotic. For example, in a strong magnetic field, the electron's trajectory becomes chaotic when the Lorentz force competes with the Coulomb binding force. Similarly, in the presence of a strong microwave field, the classical electron motion transitions from mostly regular behaviour to widespread chaos. While the solutions of the Schrödinger equations for these systems do not strictly meet the definition of classical chaos, experimental and theoretical studies have revealed a variety of new physical phenomena in the realm of quantum chaos for these simple atomic systems.

Quantum chaos is a captivating field of study that explores the intricate interplay between quantum mechanics and chaos theory. It seeks to understand the behaviour of quantum systems that exhibit chaotic classical behaviour, bridging the gap between the microscopic quantum world and the macroscopic chaos observed in classical systems. This interdisciplinary field not only sheds light on the fundamental principles of quantum mechanics but also offers profound insights into the nature of chaos and complexity in the universe.

2 Quantum Primer

At the beginning of the 20th century, it was believed that the known laws of physics were complete and could explain everything. However, the problem appeared with the observation of the atomic spectra. The series of experiments led scientists to believe that an atom consists of a positively charged nucleus and negatively charged electrons that orbit the nucleus. This model was known as the planetary model of the atom. The classical electrodynamics laws predicted that an accelerated charged particle (in this case, an electron) should constantly emit an electromagnetic wave and consequently lose energy. The loss of energy means a decrease in the electron orbit's radius and, as a result, the collapse of the atom. To resolve this issue, a new physical concept known as quantum mechanics, was introduced. This theory predicts that the electron in an atom can only have discrete energy levels, known as 'quanta.' These energy levels for hydrogen atoms were empirically found to be:

$$E_n = -\frac{1}{n^2} 13.6eV \tag{1}$$

In general, quantum mechanics tries to answer the same question as classical mechanics: Knowing a particle's position and momentum at time t, how do they evolve at time $t + \delta t$? In classical mechanics, we use either Newton's laws of motion, Lagrangian or Hamiltonian mechanics to answer this question. Unlike in classical mechanics, the position and momentum in the quantum world cannot be known to the same degree of accuracy. The uncertainty principle attributed to this field comes from the size of the objects of interest. On these scales, the effects of the wave-like nature of particles start coming into play and result in the uncertainty of the measurements of the position and momentum to the degree of

$$\Delta p \Delta x \geq \frac{\hbar}{2}$$

Where Δp and Δx are the uncertainties in the momentum and position of a particle. Therefore, quantum mechanics is a probabilistic theory which can be described by the wave function $\Psi(\mathbf{r}, t)$ and governed by the analogue of Newton's second law, which is called the Schrödinger equation:

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \hat{H} \Psi(\mathbf{r}, t) \tag{2}$$

where Hamiltonian

$$\hat{H} = \frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \tag{3}$$

is the linear operator. The linearity of the Hamiltonian results in the superposition principle in quantum mechanics and is responsible for the wave-like nature of the solutions of Schrödinger's equation. In this paper, we mainly deal with time-independent Hamiltonian so that the time-independent Schrödinger equation might be rewritten as:

$$\hat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r}), \Psi(\mathbf{r}, t) = \psi(\mathbf{r}) e^{-\frac{iEt}{\hbar}} \tag{4}$$

Where E is the system's energy. Equation 3 enables us to solve for the time evolution under the known initial wave function ψ_0. In this sense, quantum mechanics is fully deterministic, and the time evolution of the wave function can be found either analytically or numerically. According to Bohr's correspondence principle [2], quantum mechanics describes macroscopic systems equivalently to classical mechanics. This is achieved in the limit of $\hbar \to 0$ and the potential $V(\mathbf{r})$ fluctuating much slower than the wave function. This results in the eradication of the uncertainty principle and, as a result, the possibility of repeating the classical laws of motion.

However, quantum mechanics' determinism results in a lack of sensitivity to the initial conditions of the wave function and the observables [1]. In addition, the quantum mechanical energy spectrum is discrete, and the solutions of the Schrödinger equation restrict the system's quasiperiodic behaviour. These factors make it impossible to explain classical chaos from the point of view of quantum systems. Quantum Chaos, which is the topic of this paper, refers to the quantum systems in which Hamiltonians are chaotic. One of the problems that laid the foundation of quantum chaos is the problem of the energy levels of atoms under the influence of the strong magnetic field.

2.1 Classical Hydrogen atom and Zeeman effect

At the beginning of this section, we introduced the idea that the energy levels of the hydrogen atom were empirically found to be 1. This same problem can be solved analytically by noting that the Hamiltonian for this problem is

$$\hat{H} = -\frac{\hbar^2}{2m_e} - \frac{Ze^2}{4\pi\epsilon_0 r} \tag{5}$$

Where m_e is the mass of the electron, and the second term is the Coulomb's potential energy. The solution for the energy spectrum from equation 4 with the Hamiltonian from 5 is

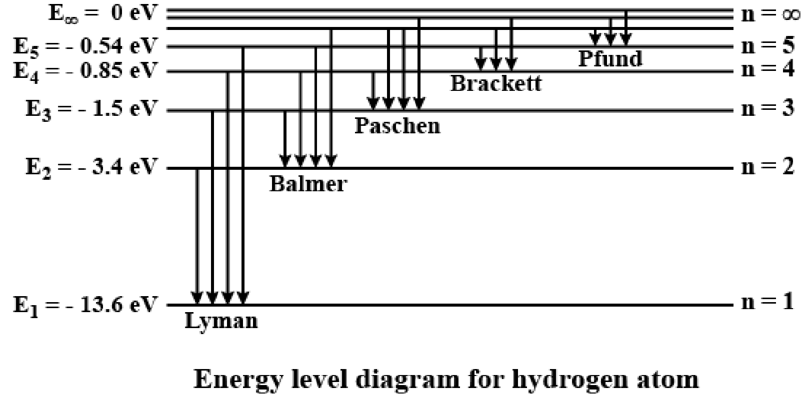
$$E_n = -\frac{1}{2n^2}\left(\frac{Ze^2}{4\pi\epsilon_0}\right)^2\frac{m_e}{\hbar^2} \tag{6}$$

When the constants are plugged into equation 6, the obtained result is exactly the equation 1.

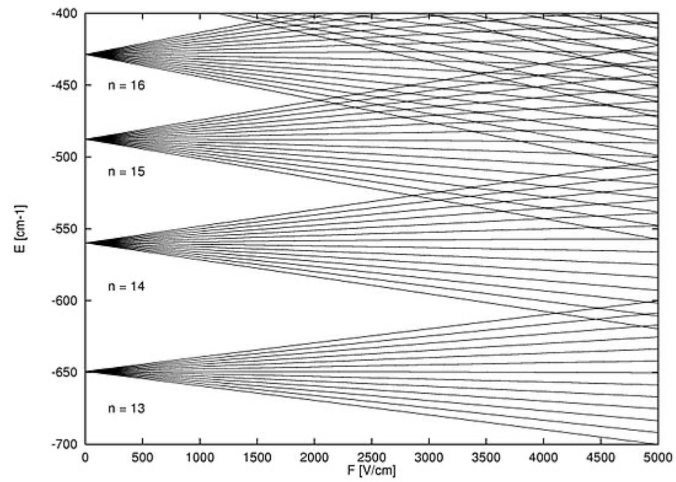
Now, think about what happens if the external magnetic field is applied to the atom. From electrodynamics, we know that a hydrogen atom has a magnetic moment $\boldsymbol{\mu}$. As a result, the applied magnetic field acting on the atom perturbs the original Hamiltonian. This perturbation is

$$\hat{H}'_z = -\boldsymbol{\mu}\cdot\mathbf{B} \tag{7}$$

This effect is called the Zeeman effect. The resulting Hamiltonian is the sum of equations 5 and 7. The result of this interaction is the splitting of the energy states, as shown in Figure 1.



(a)



(b)

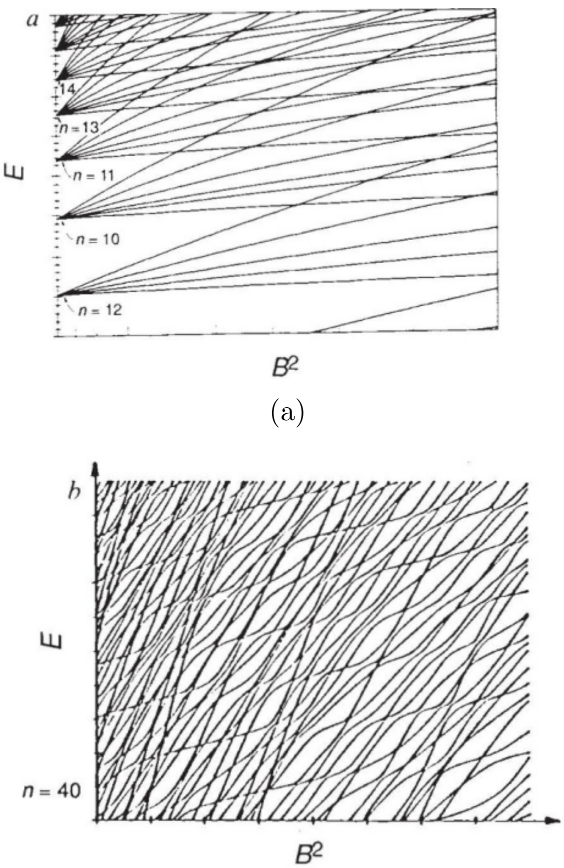
Figure 1: Hydrogen energy levels: 1a: energy levels from eq.6; 1b: perturbed energy levels by the Zeeman effect

3 Quantum Chaos

As mentioned previously, Quantum Chaos arises as a sub-study of quantum mechanics that seeks to satisfy Bohr's correspondence principle: The expectation that quantum systems coincide with classical systems in the macroscopic limit. The current methods of quantum mechanics derived from canonical quantization restrict these systems to behave quasi-periodically and have discrete energy spectra [1]. Naturally, this presents the issue that we cannot expect to find chaotic behaviour in such systems, contradicting the correspondence principle.

The study of Quantum Chaos, or more accurately, Quantum Chaology [1], serves to relieve the issue presented by this contradiction by attempting to derive classically chaotic behaviour from quantum mechanical systems. However, it should be noted that this theory is still fresh and in development, hence the reluctance to deterministically call it Quantum Chaos instead of Quantum Chaology[1]. Thus, the topics of this section will serve to introduce the working theories and experimental discoveries behind the subject.

Determining whether quantum systems can exhibit chaotic behaviour requires the examination of strongly coupled non-linear oscillators. A particular system of interest is the hydrogen atom in a strong magnetic field. As discussed previously, the hydrogen atom in a magnetic field experiences linear splitting in its degeneracy levels, according to the Zeeman effect and Perturbation Theory. However, through studies at The University of Bielefield and Massachusetts Institute of Technology, it had been discovered that when the magnetic field is comparable in magnitude to the coulomb binding field, perturbation theory fails to describe the behaviour of these energy levels[1]. Instead, what is observed in this system is an unpredictable and aperiodic splitting of the energy levels, clearly demonstrating what is classically described as chaotic. Figure 2 shows the irregular behaviour of the energy level splitting of the hydrogen atom subjected to a strong magnetic field. The threshold for the characteristic chaotic behaviour of the hydrogen atom in this configuration arises when the atom is highly excited, thereby reducing the Coulomb binding field in proportion to $1/n^4$, and allowing for lower magnetic fields to perturb the system irregularly [1]. In the ground state, much stronger magnetic fields are required to achieve this kind of behaviour (to the order of 10^4)[1]. Thus, as is shown in Figure 2b, Chaos is readily observable in excited states around $n = 40$, where the magnetic field required to perturb such a system is to the order of a few teslas[1].



(a)

(b)

Figure 2: Hydrogen energy levels perturbed by Zeeman effect: 2a:small n-nonchaotic; 2b: large n - chaotic.

While the mathematics of Quantum Chaos are still in development, primarily due to canonical quantization being incapable of satisfying the correspondence principle, the statistics of the discoveries seem to agree with what is called Random Matrix Theory (RMT). "The main goal of the Random Matrix Theory is to provide an understanding of the diverse properties (most notably, statistics of matrix eigenvalues) of matrices with entries drawn randomly from various probability distributions traditionally referred to as the random matrix ensembles"[3]. This is an initially striking proposition since the Hamiltonians of quantum mechanics seem to have no unknown or random quantities. However, when these chaotic properties of such quantum systems as the hydrogen atom in a strong magnetic field arise, RMT becomes necessary for describing the observed spectra in terms of its statistical properties of the eigenvalues [4]. RMT will not be discussed in depth in this paper due to its complexity and the fact that it is still not a fully developed theory. Nevertheless, it is useful to understand the implications of Random Matrix Theory, which can be described using the analogy of the chaotic behaviour of billiard balls on a billiard table: "The random elements describe random couplings between the various degrees of freedom. This idea goes back to Wigner and a simplified picture of Bohr, who thought of the scattering process between a hadron and a heavy nucleus as a classical billiard-ball-like game" [5]. The billiard system is used to illustrate how an object in a two-dimensional space behaves when restricted to a particular constraint. In certain circumstances, the ball moves in regular patterns, whereas slight changes in the boundary of its constraint can lead to irregular, chaotic patterns. Figure 3 shows how a circular billiard system behaves in a regular pattern, whereas slightly changing the boundary to be a cardioid leads to the chaotic motion of the billiard ball. P is the Poincaré section, defined by the boundary of the constrained motion [5].

What this implies for quantum systems and their connection to RMT is that when the initial conditions

of the system are slightly varied, they should exhibit aperiodic fluctuations in energy levels, which is exactly what is observed in the case of the hydrogen atom in a strong magnetic field. Modern studies of quantum chaos delve into the behaviour of Many-Body Quantum Chaos (MBQC), which can also be described with Random Matrix Theory and, thus, the billiard ball analogy. As mentioned previously, the study of random matrix theory is far too complex for the scope of what this paper intends to achieve. Therefore, the main focus will be placed on the general statistical properties of eigenvalue spectra and the connection between quantum chaos and classical chaos via the Lyapunov exponent.
The necessity of analyzing the statistical properties of such quantum systems comes from the fact that there are far too many energy levels to discuss each of their behaviours individually. For this reason, it is important to take note of some useful quantities that help describe these systems. Notably, the expression

$$P(s) = e^{-s} \tag{8}$$

is the Berry-Tabor conjecture, which describes the distribution of energy spacing in a given integrable system [4]. Here, s represents the level spacings which are described as

$$s_i = e_{i+1} - e_i$$

where e is the rescaled energy

$$e_i = \bar{n}(E_i)$$

and $\bar{n}(E_i)$ is described as the average number of energy levels below a given energy E_i [4]. Figure 4 demonstrates equation 8, which depicts the distribution of the energy levels of systems that exhibit non-chaotic, regular behaviour.

This means that at low excited states, the hydrogen atom in a magnetic field should have an exponentially decaying distribution.

$$\mathcal{P} := \{(s,p) \mid s \in [0, |\partial\Omega|],\ p \in [-1,1]\} \quad .$$

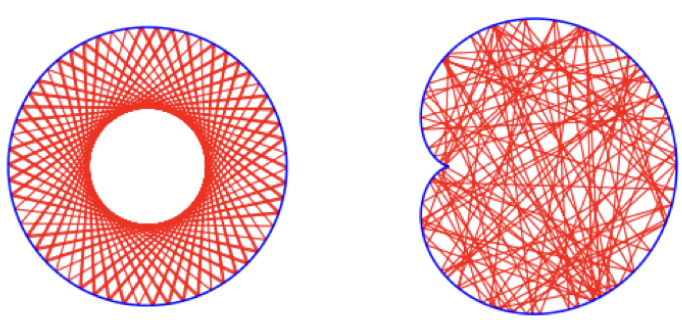


Figure 3: Behaviour of the billiard system in a circular region (left) vs in the cardioid (right)

In the chaotic regime, it is necessary to invoke different relationships that describe these systems, since it is expected that they will not exhibit regular spacings between energy levels. For these, the Bohigas-Giannoni-Schmit conjecture is used such that the probability distribution is described as a Gaussian curve:

$$P_{GOE}(s) = \left(\frac{\pi}{2}\right) se^{-(\pi/4)s^2} \tag{9}$$

Where GOE stands for the Gaussian Orthonormal Ensemble, derived from Random Matrix Theory [4]. The Bohigas-Giannoni-Schmit conjecture is a universal description of the chaotic spectra of time-reversal invariant systems. Figure 5 shows the particular distribution of the hydrogen atom in a strong magnetic field (solid curve) compared to the hydrogen atom's more regular distribution in a weaker magnetic field (dashed line). What this means for the system is that the energy levels are unlikely to cluster (s=0), meaning the energies cannot be described in the normal quantum mechanical sense which predicts that the split energy levels result from a dispersed perturbation of quantized energy levels is equation 1
Instead, the energy levels have a scattered probability distribution according to the Gaussian curve and are much more likely to have larger separations in energy levels. This means that energy levels are strongly repelled from each other when chaotic behaviour ensues.

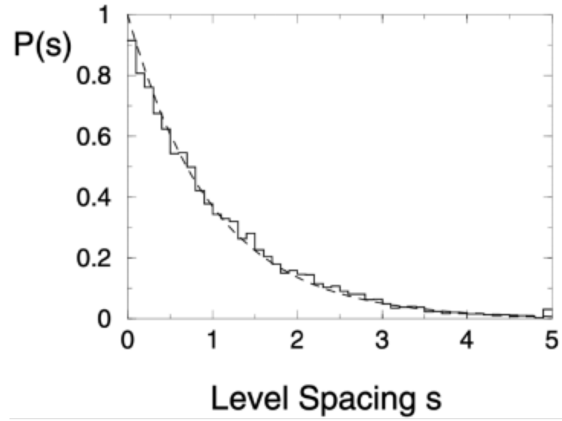


Figure 4: distribution of energy levels vs level spacing in non-chaotic systems.

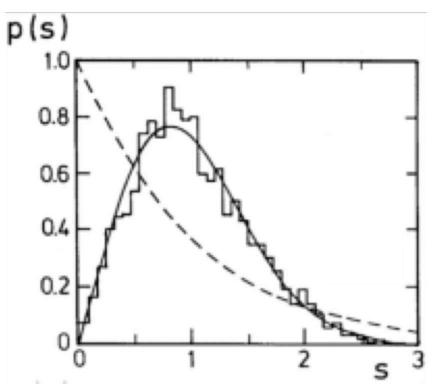


Figure 5: distribution of energy levels vs level spacing in non-chaotic systems,

A modern field of study in the realm of Quantum Chaos is the study of the behaviour of black holes. Black holes are said to be an extremely chaotic phenomenon due to their tendency to destroy information very quickly and have immense increases in entropy, exhibiting very high temperatures [4]. The most important contribution from this field of research is in the development of the Sanchdev-Ye-Kitaev (SYK) model, which describes "maximally" chaotic thermodynamic systems such as the black hole [4]. Furthermore, Maldacena argues that from this model, we may extract a quantum equivalent to the Lyapunov exponent: "Maldacena proposed a conjecture that using statistical mechanics quantities like the thermal expectation values of a commutation of Hermitian operators, or other related quantities (via traces, etc.) lead to a bound on chaos for all thermal quantum systems with many degrees of freedom (not just black holes)" [4]. The exponent, much like in classical chaos, describes the exponential divergence from initially neighbouring trajectories.

$$\lambda_L \leq 2\pi T \tag{10}$$

Due to the chaotic thermodynamic description of black holes, the system is comparable to the discussed system of a hydrogen atom in a strong magnetic field which exhibits chaotic disorder in its energy levels. Thus, this quantity (equation 10) can be considered as the quantum chaos equivalent of the Lyapunov exponent. Moreover, it provides a measure for determining the degree of energy level repulsion demonstrated in the Gaussian probability distribution as seen in Figure 5, particularly for the large separation at the minimally perturbed energies, when energies should classically intersect.

4 Applications

Quantum chaos explains experimental results, such as the behaviour of atoms in a strong magnetic field, and has applications across various scientific fields. In the modern world, the development of new computational apparatus could lead humanity into a new era of science. Quantum computers are being developed all over the globe and might become the next major breakthrough since the development of classical computers. Unfortunately, scientists must overcome many challenges before these machines can perform on the same level as transistor computers. One such challenge is resolved using Quantum Chaos.

Quantum Computers operate on principles of quantum mechanics, using quantum bits (qubits) to perform computations. The biggest difference between the bits and qubits is that the former can represent either 0 or 1, while the latter can be a 0 and a 1 simultaneously due to the superposition principle described above. The computational power of a computer comes from the number of bits it can simultaneously store. The higher the number – the better the computer. However, in quantum computers, the large number of particles results in chaotic behaviour (similar to quantum billiards), which might cause significant errors when interpreting the stored data. The theory of quantum chaos is used to resolve this issue by introducing quantum error correction. This correction uses the theoretical foundations of quantum chaos, which were described in the previous section, to account for the chaotic behaviour and reduce the errors. This is crucial for fault-tolerant quantum computers.

Cryptography can also be enhanced by quantum chaos. Cryptography is used to secure information by encoding it with random numbers. The ideal random number is one that cannot be predicted under any circumstances. However, computer-generated random numbers are imperfect and depend on the code that creates them. To address this, people are utilizing various naturally occurring phenomena to generate random numbers. For instance, Cloudflare uses a wall of lava lamps to aid in encryption. In the future, the study of quantum chaos could be used to encrypt information by leveraging the randomness of quantum processes.

Quantum chaos can also be applied to theory. For instance, as mentioned before, quantum chaos can explain the vanishing information in black holes. It can also be used to develop high-temperature superconductors, which can make the world look like a fantasy from the 1950s. Quantum chaos can be used to study mesoscopic systems. These systems are intermediate in size between microscopic and macroscopic and, due to their quantum nature, exhibit chaotic behaviour, such as conductance fluctuations and persistent currents. Quantum chaos is used to explain all these phenomena and aids scientists in the creation of new materials.

Overall, quantum chaos is used in a wide variety of fields. It can help us build new and powerful quantum computers, develop new materials, and explain phenomena that cannot be explained either by quantum mechanics, classical mechanics, or chaos. But, combined together, quantum mechanics and chaos can give us a new and better world.

5 Conclusion

In summary, quantum chaos is a fascinating field that explores the unpredictable nature of quantum systems despite their deterministic foundations. It challenges the idea of perfect predictability in quantum mechanics by showing that quantum systems can behave chaotically, similar to classical chaotic systems.

This field has practical applications in quantum computing, cryptography, materials science, and the study of complex systems. By delving into the behaviour of quantum systems exhibiting chaotic classical behaviour, quantum chaos offers profound insights into the complexity of the universe. Quantum chaos is an interdisciplinary field that enriches our understanding of quantum mechanics and has the potential to revolutionise various aspects of science and technology. It continues to unravel the mysteries of the quantum world, opening doors to new discoveries and innovations.

References

[1] Jensen, Roderick V. (23 January 1992) *Quantum Chaos*, Nature Publishing Group.

[2] Bohr. N. (1918) Kgl. Danske Vid. Selsk. Skr. nat-math. Afd. 8. Raekke IV.1. 1-3: (reprinted) in *Sources of Quantum Mechanics* (ed. van der Waerden, B. L) 95-137 (Dover, New York, 1967).

[3] Fyodorov, Yan. (3 March 2011) *Random Matrix Theory*, Scholarpedia. Acquired on 30 March 2024 from `http://www.scholarpedia.org/article/Random_matrix_theory`

[4] Korolev, Magali. (February 2023) *An Introduction to Quantum Chaos*, International Centre for Fundamental Physics. P. 8 - 20.

[5] Bäcker, Arnd. (n.d.) *Quantum Chaos in Billiards*, Institut für Theoretische Physik. P. 1 - 2.

[6] Sandro Wimberger (2013) *Nonlinear Dynamics and Quantum Chaos. An Introduction*, Springer International Publishing Switzerland