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Quantum Effects in Biological Systems: Enzymatic Reactions & Photosynthesis

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Abstract: ***In the emerging field of quantum biology, we begin to see how biological systems exploit quantum mechanics as their efficiency and certain phenomena such as photosynthesis and enzymatic reactions cannot be explained only by classical physics. This paper will shortly review the foundations and axioms of quantum mechanics including wave particle duality, Heisenburg's uncertainty principle and the probabilistic interpretation of a wave function before exploring the first primary topic- quantum tunneling in enzymes. The paper will then provide deeper insights into quantum effects in photosynthesis including coherence, entanglement and the photoelectric effect. Additionally, quantum biology will have profound implications on the future of quantum technology. Leveraging the information scientists have gained about the quantum mechanical functions of biological systems, this paper will delve into the applications of this know-how in quantum technology.***

Keywords: quantum biology, quantum mechanics, photosynthesis, enzymatic reactions, quantum technology

1. Introduction to Quantum Physics

1.1 The History of Quantum Mechanics

Quantum mechanics was discovered when a number of observations that could not be explained by classical physics emerged. Max Planck, a German physicist, produced the original quantum theory which was later refined by Niels Bohr, Erwin Schrödinger and Paul Dirac amongst others. Planck was initially fascinated by how energy was radiated from objects based on wavelength. Upon experimentation, the physicist announced 'Planck's radiation formula' and introduced the notion of 'quanta'- discrete packets of energy. According to planck, the higher the temperature of an object, the higher the energy emitted and so the higher frequency emitted. This notion was the world's first insight into quantum theory and was deemed one of the most revolutionary discoveries in the history of physics.

As aforementioned, quantum theory was refined by many physicists, namely Niels Bohr. Bohr helped develop the model of the atom which showed that there were multiple concentric shells containing electrons and that electrons move between energy levels when they absorb or emit radiation causing the atom's energy state to change. Upon observation of the electrons, Bhor discovered phenomena which defied Newtonian laws. He observed that electrons could be in multiple places at the same time and that electrons were subject to wave particle duality. Furthermore, Bhor found that until electrons were measured they could be in a superposition of states- meaning they could be in mutually exclusive states at the same time. This led to the development of old quantum theory and propelled physicists further into the realm of quantum mechanics.

1.2 Classical vs quantum physics

Quantum mechanics first emerged when physicists realized that they were unable to explain dynamics at a subatomic level. As such, Newtonian laws did not apply to microscopic scales, leading to the laws of quantum mechanics. More specifically, the realm of quantum physics was discovered by German physicist Max Planck who originated old quantum theory and developed Planck's equation to explain the relationship between frequency and the size of energy packets.

In quantum mechanics, phenomena occur at ultrafast time scales like chemical reactions, for example the combustion of hydrogen has a flame speed of 1.7 m/s.

When molecules collide there is potential energy between them and the molecules must collide with enough kinetic energy to overcome this barrier. However, in quantum mechanics a phenomenon called quantum tunneling occurs. This means that molecules can 'tunnel' through this barrier without needing to overcome it. [1] An instance of this 'tunneling' can be shown when the shuttlecock goes through the racket instead of bouncing back. This results in an extremely high rate of reactions which can be calculated using Schrodinger's equation. Thus, phenomena in quantum mechanics occur at faster time scales.

1.3 Heisenberg's uncertainty principle

This principle states that the position and momentum of a particle cannot be known at the same time. The more you work on one value, the less you will know about the other. While determining the position of the particle a photon from the measuring device collides with the particle, so some of its momentum is transferred to the particle, making the value of momentum inaccurate [2]. The value of position will also be inaccurate because the photon will cause the particle to move from its original position.

The uncertainty principle is essentially due to the fact that subatomic particles display wave particle duality. Hence, there is a probability of position being in a range of different places. The more precise the position of the wave is the more inaccurate the wavelength. This means that velocity is imprecise and hence, so is momentum [3].

Heisenburg's uncertainty principle can be mathematically explained with matrices. As aforementioned, the momentum position uncertainty principle states that the more you learn about momentum the less you know about the position of the particle and so you can't measure both values simultaneously.

Operators are used in order to measure physical observables. When these observables commute and the value of the commutator is zero then you can simultaneously measure the observables. This is because they have the same eigen basis. However, in quantum mechanics, generally matrices do not commute and cannot be measured simultaneously. As such, these observables have an uncertainty relationship. Meaning, if you investigate v_1 further you will know less about v_2. The superposition of v_1 and v_2 can be shown by multiplying an eigen value by the sum of the eigenvectors of v_1 and v_2 as demonstrated below.

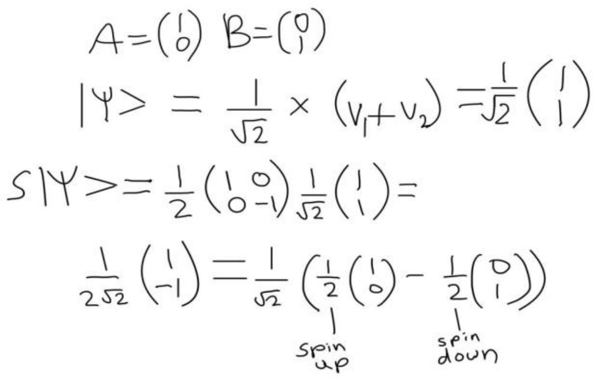

Figure 1: Mathematical Explanation of Matrices

Sz refers to the spin operator, v_1 & v_2 refer to the states while Ψ refers to the superposition of states.

In Heiseburg's uncertainty principle, position and momentum have the commutator [x^,p^]=i$\hbar$ and so cannot be measured simultaneously due the lack of the same eigenbasis. Hence there is an uncertainty between position and momentum.

1.4 Schroedinger's cat

This is a thought experiment where you have a cat in a box with poisonous gas and has a chance of killing the cat 50% of the time and 50% of the time nothing happens. Because the survival of the cat is probabilistic, before looking inside the box the cat is in a superposition of states- it is both alive and dead. This is because there is no conscious observer. However, once the box is opened, the system collapses into reality and the cat is either dead or alive. This thought experiment is essentially a representation of the behavior of subatomic particles in quantum physics. Before observation, there is a superposition of wave functions just like how the cat is in a superposition of the 'dead' wave function and the 'alive' wave function. However, when observed the wave function collapses and there is only one state, similar to how the cat is only dead or alive [4].

1.5 Double slit experiment

This experiment demonstrates wave particle duality as it shows that light behaves like a wave. If light would behave like a particle then you would predict that there would be two strips on the screen where the slits are. However, the pattern observed on the screen consists of alternating dark and light fringes. This is because when light passes through the slits it diffracts and the waves interfere with each other. Where the peak of a wave lines up with the peak of the other wave, constructive interference occurs. However, where the peak of a wave lines up with the trough of another wave destructive interference occurs. Constructive interference essentially occurs when there is a phase difference that is a multiple of 2π and destructive interference occurs when waves are in antiphase. The production of the dark fridges is due to destructive interference while the production of the light fridges is due to constructive interference. The fact that interference and diffraction are both being demonstrated shows that light behaves like a wave.

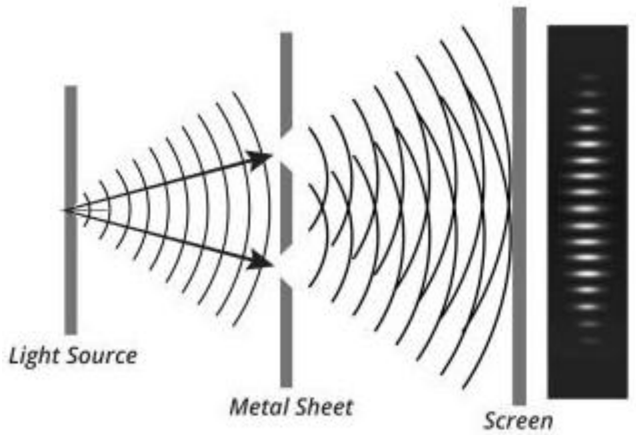

Figure 2: Double Slit Experiment (based on https://www.discovery.com/science/Double-Slit-Experiment)

1.6 The photoelectric effect

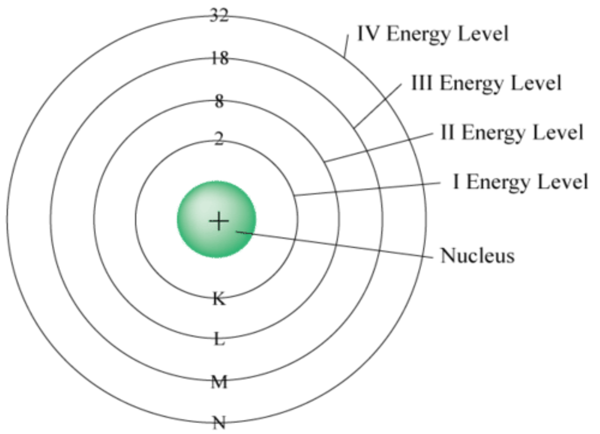

Figure 3: Electron Shells (based on https://flexbooks.ck12.org/cbook/ck-12-chemistry-flexbook-2.0/section/5.12/primary/lesson/energy-level-ms-ps/)

The photoelectric effect demonstrates the concept of wave particle duality as light behaves like a particle in this phenomenon. An atom has a number of fixed energy levels and movement between this involves the absorption and emission of a photon. Only a photon with certain energy could cause an electron to 'jump' between two energy levels. This shows that light behaves like a particle because if it were to act like a wave, with time energy would build up and cause the emission of the electron. Furthermore, the emission of electrons is instantaneous, with waves it would take time for the energy to build up and so it would take time for the electrons to be released. Furthermore, if light were a wave, as intensity would increase so would kinetic energy. However this is not the case, as intensity increases only the number of photons emitted per second increases.

1.7 Probability Interpretation of Wave Function

Lets, say you have a ball on a floor and you measure the position of the ball. Next, you place the ball in the same position and measure it again, you will get a different value each time due to uncertainty. This distribution can be displayed through a diagram. Plot p(x) on the y axis and x on the x axis. According to physicists, p(x) is related to the modulus of psi of x squared.

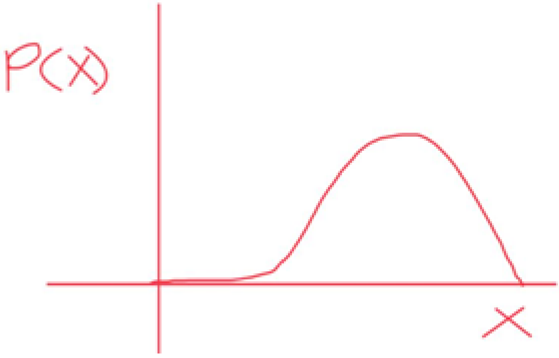

Figure 4: Probabilistic Distribution

If a system is a single particle, the wave function is directly related to getting the probability of the experimental result when making a measurement on a system so the wave function is directly related to finding the particle in a different position. The wave function is represented by psi. More specifically, the square modulus of wave function is related to the probability of finding a particle at a certain point. To determine the value for this probability, plot a graph of psi on the y axis- as it's thought to be the probability distribution for the position measurements- and x on the x axis. Then plot a graph of the absolute value of the wave function squared. Then calculate the probability that a particle will be found between two points by finding the integral of modulus psi squared between these two points [5]. This will give you the area which will in turn give you the probability. As such, where the area is greatest, so is the probability. As depicted in Fig. 5.

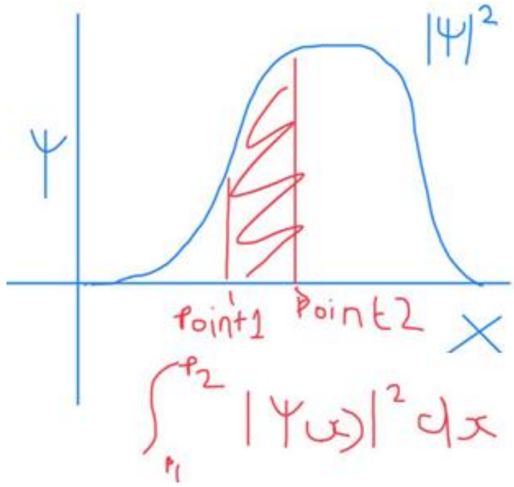

Figure 5: Value of Probability

After measurement is taken the graph of wave function before is wide and afterwards it's narrow as depicted in Fig. 6. This shows that the wave function has collapsed. Similar to the aforementioned cat experiment, there is now only one state- the cat is either dead or alive and no longer in a superposition of both states.

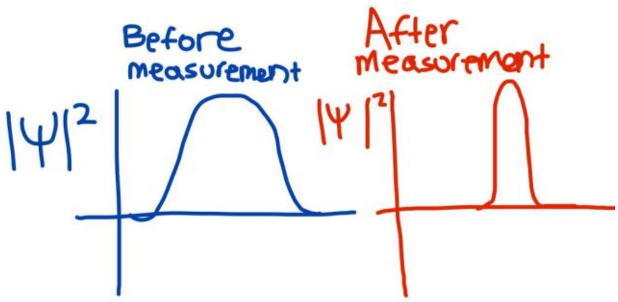

Figure 6: Collapse of wave function

2. Quantum effects in biological systems

2.1 Quantum coherence & the Photoelectric effect

Photosynthesis is the renowned fundamental process that converts light energy into chemical energy to produce glucose. The chloroplasts contain thylakoid which contains the pigment chlorophyll that is responsible for this process. Chlorophyll has a single valence electron that is ejected when a photon- quantized packet of energy- collides with an antenna which is a light harvesting protein-pigment complex and is absorbed by the chlorophyll. This is due to the aforementioned phenomenon- the photoelectric effect. Most leaves absorb only the green wavelength as this specific wavelength will trigger the loss of the electron [6]. This leads to charge separation. The transfer of the electron leaves behind a positively charged space are paired with each other to form an exciton which is then transferred in the antenna to reach the reaction center which consists of multiple pigments and proteins that initiate the conversion of energy [7].The exciton travels towards the reaction center to produce ATP from sunlight, producing chemical energy [8]. There are a variety of different paths but the photon is not aware of which one is most efficient. Hence, this is where quantum coherence is believed to come into play as the photon travels down all paths at the same time, finding the best route. This explains the extremely efficient transfer of solar energy- almost all photons contribute to chemical energy- to the reaction center instead of accounting for the ultrafast speed via an energy gradient. However, this was initially hard for scientists to believe due to decoherence. Normal quantum reactions take place at absolute zero temperature and in isolated conditions to avoid measurement and decoherence. Thus, it was surprising that such reactions could occur in the conditions of the environment [9]. However, experiments conducted showed an interference pattern in which that quantum superposition was taking place. Furthermore, it was first believed that the excitons were randomly passed on to other pigments until reaching the reaction center but this did not account for the extreme efficiency of photosynthesis making the quantum theory more viable. Each chlorophyll molecule is at a different energy state and when a photon is absorbed it was believed that the vibration was passed onto a series of molecules with lower energy levels until reaching the reaction center.

Another theory of where quantum effects come into play is when light energy is absorbed by chlorophyll the energy is shared between all chlorophylls at once due to quantum superposition. As a result the efficiency is much greater as more photons are absorbed at the same time and almost every photon of the captured solar energy is used by the cell [10].

On the other hand, the classical belief is that the efficiency in photosynthesis is due to vibrations. In some studies, researchers observed that the protein PC645 can control the route of the absorbed light energy to encourage energy transport via certain routes. This means that the excitation is only passed on to certain pigments only. Additionally, the excitation is only shown to be at the highest energy level or the lowest energy level and not at any energies in between. Some researchers believe that this is not due to quantum mechanics, but instead by a 'large band of vibrations that bridge the energy gap between two pigments' [11].

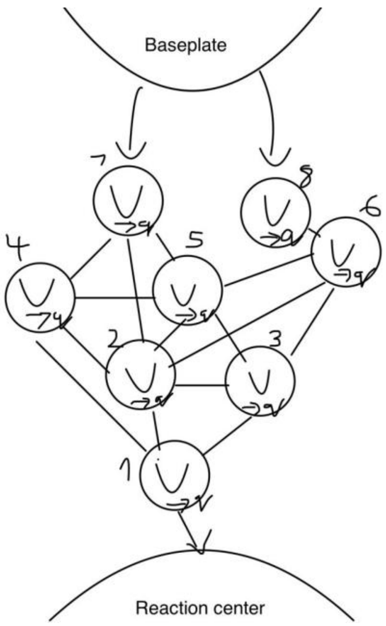

Figure 7: Transfer of Energy from baseplate to Reaction Center (based on https://pubs.acs.org/doi/10.1021/acs.jpclett.2c00538)

The circles on the diagram represent different excitonic states and the parabola stands for the energy function. Furthermore, the connecting lines represent the coupling between the energetic states. There are multiple lines going in different directions to showcase the different possible routes of the vibrational energy.

It is remarkable that such quantum reactions can take place at room temperature due to thermal energy which would result in noise. When observing quantum effects the system is very simple and normally consists of one single molecule. However, biological systems are made up of many molecules with various degrees of freedom. Thus, environmental conditions are thought to be unfavorable for quantum reactions as thermal energy kT will overpower the actions of the photon. But if the notion that photosynthesis is governed by quantum mechanics is true then it would seem that the environment is not hindering, but instead facilitating the process.

2.2 Quantum Entanglement in Photosynthesis

Quantum entanglement refers to a group of particles where the quantum state of each particle cannot be described independently from each other. Essentially when you measure the state of one you will know the state of the other. Particles that are quantumly entangled will change state simultaneously regardless of the distance between them.

According to Quantum entanglement in photosynthetic light-harvesting complexes (Sarovar, M., Ishizaki, A., Fleming, G. *et al* 2010), Quantum entanglement may be important in multichromophoric light-harvesting complexes. They describe entanglement as the 'non-local correlation between electronic states of spatially separated chromophores' and the excitation state as a superposition of chromophore sites in excited states and ground states. Essentially, in the simplest scenario when one chromophore is excited the rest are in ground state. Thus if you measure the excited chromophore you will immediately know the rest are in ground state. Quantum entanglement may be behind the near 100% efficiency of photosynthesis [12].

2.3 Quantum tunneling in Enzymatic Reactions

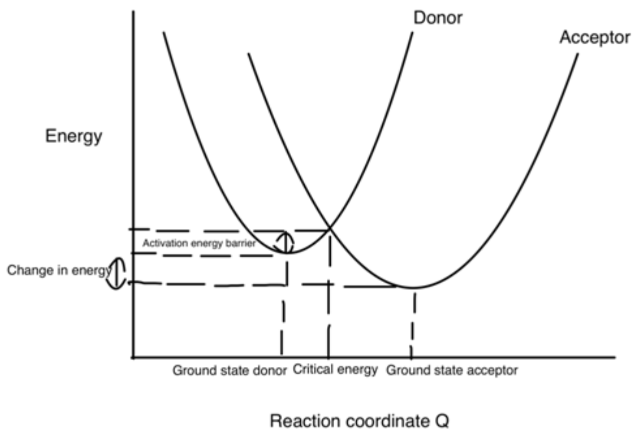

Figure 8a

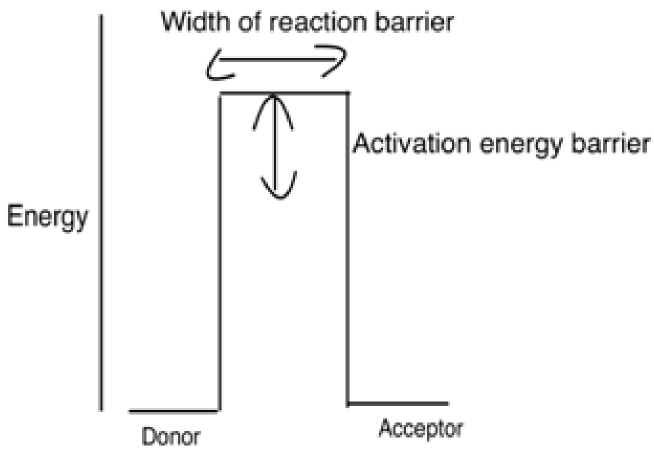

Figure 8b

Enzymes are essentially biological catalysts that increase the rate of a reaction without being used up by lowering the activation energy required for an enzymatic reaction to occur. Enzymes operate via a lock and key mechanism. Each enzyme can only bind to a specific substrate due to the shape of its active site. Generally, in enzymatic reactions the greater the temperature the greater the rate of the reaction. This is because the kinetic energy of the molecules increases, raising the likelihood of forming an enzyme substrate complex. However, experiments conducted by scientists DeVault and Chance showed that while this relationship was present at higher temperatures, at low temperatures like 100-4k this temperature-activity correlation was no longer applicable [13].At such temperatures the rate of the reaction was significantly higher, which no longer could be explained classically suggesting that the phenomenon of quantum tunneling was taking place.

In figure A, the energies for the donor and acceptor are displayed by the curves. One can think of the two ground states as two valleys. When going from one valley to the other, one has to climb a hill or a mountain. In this scenario the ground state of the donor is higher than the ground state of the acceptor. The critical point is the intersection of the curves; this is deemed as the critical point because slight movement to the left would cause the ball to fall down to the donor, similarly movement to the right would cause the ball to fall down to the valley of the acceptor. The change in energy is the difference in energy between the ground states of the acceptor and donor and in this scenario could be demonstrated as the net height difference between the two valleys. The ball must roll from the point of the ground state on the acceptor to that of the donor. Then the molecules must overcome the activation energy in order for the reaction to occur, which is the barrier that needs to be overcome by climbing from the starting point in the valley to the critical point. If the ball rolled from the ground state of the acceptor to that of the donor, this would be an endothermic reaction as energy is required. If the ball rolled from the ground state of the donor to that of the acceptor, that would be an exothermic reaction as energy is released.

While figure A is a classical representation, figure B is a quantum interpretation. In classical physics the only quantity that would matter is the value of the activation energy barrier. However, according to figure B the width of the barrier is also important. This is because in quantum mechanics molecules 'tunnel' through instead of actually overcoming the barrier. The probability of quantum tunneling depends on the width of the activation energy barrier. The greater the width, the lower the probability of quantum tunneling, vice versa.

3. The Future of Quantum Biology

The knowledge acquired when studying quantum mechanical effects in biological systems will give us a better understanding of these processes and this newfound understanding can be applied to quantum technology in the future. Quantum mechanics helps such systems achieve extreme efficiency and speed- qualities that can be used to advance our modern day gadgets including solar panels and batteries.

Some applications of quantum biology include incorporating quantum mechanical design into solar cells to increase efficiency, essentially using light harvesting for energy generation. Furthermore, according to the paper Photosynthetic energy transfer at the Quantum/Classical Border (2018)- 'advances in the field and suggest that photosynthetic processes can take advantage of the sensitivity of quantum effects to the environmental 'noise' as means of tuning exciton energy transfer efficiency. If true, this design principle could be a base for 'nontrivial' coherent wave property nano-devices.' [14].

The current issues with manufacturing commercial quantum computers are the conditions required to maintain the computer- like near zero temperatures & isolation- and the problem of quantum noise. However, quantum mechanical effects are taking place in the conditions of biological systems which are noisy and still appear to be fine tuned. As such, if scientists can study and emulate the conditions for biological quantum systems it may be possible to apply this know-how to quantum computers. Additionally, the problem of scalability may also be resolved as more qubits will be able to be utilized in the production of quantum computers. Currently it is only possible to use up to 50 qubits due to their sensitivity which often leads to decoherence and so it is impossible to simulate circuits once the number of qubits exceeds 50 [15]. Hence, the study of such biological systems will propel us towards producing the world's commercially viable quantum computer.

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