Quantum Neural Processing

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Abstract

This paper discusses a possible neural qubit, the Posner molecule, and how it can cause quantum effects on cognition. First, previous evidence of quantum effects influencing cognition are discussed, along with the properties necessary for a neural qubit. Next, the specific properties of Posner molecules, such as nuclear spin coherence time and how entanglement between individual molecules causes entangled chemical reactions, are discussed. Finally, the impact of Posner molecule uptake by neurons on their firing rate is discussed, along with the possibility of neuronal entanglement.

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1 Introduction

It is commonly believed that quantum processes play no role in the human brain, as maintaining coherence for longer than seconds in an aqueous environment is extremely unlikely. While quantum mechanics describes the activity of individual ions and small molecules, these structures will interact with the surrounding environment and cause any possible quantum effects to go out of phase with each other and decohere. However, in 1986, researchers at Cornell University examined the effects of two different lithium isotopes, lithium-6 and lithium-7, on female rats. The rats were split into four groups: a control; one that was fed lithium-6; one that was fed lithium-7; and one that was fed pharmaceutical lithium, which contains mostly lithium-7. While the rats were consuming lithium, they were impregnated, and after giving birth, were observed caring for their young. Rats that were fed either lithium-7 or pharmaceutical lithium showed lower levels of maternal behavior, like nest-building and grooming their young, than the control group, while the rats that were fed lithium-6 showed higher levels of maternal behavior than the control group. Therefore, these two isotopes, which differ by just one neutron, had opposite effects on rat behavior, suggesting a possible quantum influence on neural activity. [1]

2 Nuclear Spin Coherence

The single-neutron difference between lithium-6 and lithium-7 impacts both the atomic mass and nuclear spin of each isotope. While lithium-7 is slightly heavier, in the brain, lithium is encased in a shell of water molecules that is significantly heavier than either isotope. On the other hand, lithium-7 has a nuclear spin of $\frac{3}{2}$ while lithium-6, due to its extremely weak electric quadrupole moment, behaves like an atom with nuclear spin $\frac{1}{2}$. This impacts the coherence time, as lithium-7 will have stronger interactions with the electric field generated by the nearby ions than lithium-6, and will decohere faster. In fact, lithium-7 remains coherent for only $\sim 10$ seconds, while lithium-6 will decohere after $\sim 5$ minutes, suggesting that differences in nuclear spin can influence neural activity through coherent quantum effects.

Nuclear spin ($L$) is a half-integer value that describes the spin of an atomic nucleus. [2] It is weakly coupled to the environment, which allows for quantum effects to remain coherent for more time. If $L \neq 0$, there is an associated magnetic dipole moment that precesses about the magnetic fields generated by the magnetic dipole moments of nearby atoms and molecules, and if $L > \frac{1}{2}$, there is also an electric quadrupole moment that couples to electric field gradients generated by nearby atoms and nuclei. In the brain, electric fields are the primary source of decoherence, and are also stronger than magnetic fields. Therefore, atoms and ions with nuclear spin $\frac{1}{2}$ will have the longest coherence times. $^1$

$^1$Most of the information from here on will be from [3]
3 Possible Neural Qubits

A prospective neural qubit must have a nuclear spin of $\frac{1}{2}$ in order to maximize its coherence time. Of the most common naturally occurring elements in the brain, the only one with nuclear spin $\frac{1}{2}$, besides the $H^+$ ion, or proton, is phosphorous.

In the brain, phosphorous ($P$) is bound to the the phosphate ion ($Pi$), which has the chemical formula $PO_4^{3-}$. It is found in energy storage molecules, like ATP, and poly-phosphate chains, such as the pyrophosphate ion ($PPi$), whose chemical formula is $P_2O_7^{4-}$. The molecular structure of $Pi$ consists of a phosphorous atom encased in a tetrahedral shell of four oxygen atoms, which resembles the hydration shell surrounding lithium-6 in the brain. However, $Pi$ has a spin coherence time of 1 second, as in the brain, it will bind to a proton and form monohydrogen phosphate ($HPi$) with a chemical formula of $HPO_4^{2-}$. Therefore, in $HPi$, the nuclear spins of the proton and phosphorous will interact through electrons and cause the spin to rapidly decohere. Thus, $Pi$ is unlikely to be an effective neural qubit, although it can serve as a qubit transporter, for it diffuses $\sim 10^{\mu m}$ in $10^{-2}$ seconds, while still maintaining coherence.

If another cation with nuclear spin 0 can displace the proton from binding to $Pi$, longer spin coherence times are possible. Calcium ions ($Ca^{+2}$) have a nuclear spin of 0 and naturally bound to phosphorous in bone-mineral, suggesting that there are physiological conditions where $Ca^{+2}$ is more likely to bind to ($Pi$) than protons, which would allow for longer spin coherence times.

The most likely neural qubit is the Posner molecule, $Ca_9(PO_4)_6$. Its molecular structure consists of eight calcium ions at the corners of a cube, a ninth calcium ion at the center, and one phosphate ion on each cubic face. In the brain, the magnetic fields from water molecules will cause the phosphorous nuclear spins to precess at frequencies of $\sim 10^{-3}$hz. However, Posner molecules rapidly tumble through water at frequencies near $10^{13}$hz, causing the magnitude and direction of the magnetic field acting on a phosphorous nucleus to rapidly change. Therefore, the net effect of magnetic decoherence on the phosphorous atoms in Posner molecules will average out to zero, which could increase the coherence time to about a day.

Figure 1: A Posner molecule with its symmetry axis pointing out of the page. The tetrahedral structure of the phosphate ion can also be seen in this figure. [4]
4 Qubit Entanglement

Entanglement is necessary for quantum processing. In particular, the singlet spin state

\[ |s⟩ = \frac{|↑↓⟩ - |↓↑⟩}{\sqrt{2}} \]  

(1)

is completely entangled, for if the first particle is measured to have spin up, the second particle spin must have spin down, and vice-versa. Notably, this effect will apply regardless of how far away the two particles are.

The nuclear spins of PPi can be described by a two-qubit system, consisting of the singlet state mentioned above and the following three triplet states

\[ |t_+⟩ = |↑↑⟩ \]  

(2)

\[ |t_0⟩ = \frac{|↑↓⟩ + |↓↑⟩}{\sqrt{2}} \]  

(3)

\[ |t_-⟩ = |↓↓⟩ \]  

(4)

A general nuclear spin state of PPi can be written as a linear combination of singlet and triplet spin states in the following manner

\[ Ψ_{PPi} = c_s ψ_s(\hat{r}) |s⟩ + c_t ψ_t(\hat{r}) |t⟩ \]  

(5)

\[ |t⟩ = \sum_m a_m |t_m⟩ , m = 0, ±1 \]  

(6)

The singlet and triplet states are orthonormal, \(|c_s/c_t|^2\) represents the probability that the PPi is in a singlet or triplet state, and \(\hat{r}\) is a unit vector specifying the orientation of the PPi ion.

PPi contains two phosphorous atoms, which are identical fermions. Therefore, \(Ψ_{PPi}\) must be antisymmetric when the two atoms are interchanged, which corresponds to an exchange of the spins and an 180° rotation that sends \(\hat{r}\) to \(-\hat{r}\). The singlet state is antisymmetric under interchange and the triplet states are symmetric. Therefore, to ensure that the whole state is antisymmetric

\[ ψ_s(\hat{r}) = ψ_s(-\hat{r}) \]  

(7)

\[ ψ_t(\hat{r}) = -ψ_t(-\hat{r}) \]  

(8)

If the PPi is freely rotating, its stationary states will be spherical harmonics labelled by a positive integer angular momentum \(l\). When the spherical harmonic is rotated 180°, it gains a factor of \((-1)^l\). Therefore, \(ψ_s\) can be written in terms of even angular momentum wavefunctions and \(ψ_t\) in terms of odd angular momentum wavefunctions. In water, the PPi freely tumbles with \(L ∼ 100\), so this distinction is irrelevant. However, the hydrolysis reaction

\[ PPi → Pi + Pi \]  

(9)
requires completely stopping the PPI from rotating, which likely depends on the sign of \((-1)^l\), suggesting a reaction rate that differs for singlet and triplet states.

The hydrolysis of PPI is catalyzed by the enzyme pyrophosphatase. Pyrophosphatase contains a magnesium-bound oxygen at each end of the x-axis and y-axis with a charge of +1. This will attract PPI into the enzyme and cause its rotations to slow, so the PPI will align along either the x-axis or the y-axis.

![Figure 2: A model of the pyrophosphatase enzyme, with a PPI molecule rotating inside. The PPI will be attracted to the four Mg\(^+\) ions in the enzyme, which will cause its reactions to slow.](image)

Define \(v_x\) and \(v_y\) as the strength of the potential causing the oxygens of the negatively charged PPI ion to be attracted to the magnesium-bound oxygens along the respective axis. This is also known as the pinning potential.

Consider deforming the enzyme along the y-axis. If the distance between the magnesium ions increases, \(v_y\) will decrease, and if the distance between the magnesium ions decreases, \(v_y\) will increase. If \(v_y\) is high and the PPI is aligned along the y-axis, weak chemical bonds will form between the oxygens at the ends of the PPI molecule and the magnesium ions. These bonds will weaken the chemical bonds between the phosphorous atoms and the central oxygen of PPI, driving the reaction

\[
PPi + H_2O \rightarrow 2H^+ + 2Pi \tag{10}
\]

The two phosphate ions will leave the enzyme, completing the reaction.

To see the effects of spin on this reaction, align the PPI along either the x or y axis, where it can rotate either clockwise or counterclockwise. \(\mid x_-\rangle, \mid y_-\rangle\) represent clockwise rotations with the PPI aligned along the respective axis, and \(\mid x_+\rangle, \mid y_+\rangle\) represent counterclockwise rotations. Therefore, the singlet and triplet states along each axis can be represented by

\[
\mid x_s\rangle = \frac{\mid x_+\rangle - \mid x_-\rangle}{\sqrt{2}} \tag{11}
\]
\[ |x_t\rangle = \frac{|x_+\rangle + |x_-\rangle}{\sqrt{2}} \]  

which are the same when the PPI is aligned along the y-axis. The orbital dynamics of the PPI can be modelled by the following Hamiltonian

\[
H_{s/t} = -t_{s/t} \left( |x_{s/t}\rangle \langle y_{s/t}| - v_x |x_{s/t}\rangle \langle x_{s/t}| - v_y |y_{s/t}\rangle \langle y_{s/t}| \right)
\]  

where the first term represents rotational motion and the last two terms represent the pinning potential attracting the oxygens of the PPI to the Mg\(^+\) ions along the x and y axis, respectively. Note that the Hamiltonian for the singlet and triplet states is identical.

The constant \(t_{s/t}\) in the Hamiltonian represents the rotation rate of the PPI. For the singlet state, \(t_s = t_+ + t_-\), and for the triplet state, \(t_t = t_+ - t_-\), where \(t_+\) is the rate of counterclockwise rotation and \(t_-\) is the rate of clockwise rotation. If \(t_+ = t_-\), then the triplet wavefunction cannot rotate due to destructive interference.

Deformation of the enzyme pocket, where the reaction occurs, drives the hydrolysis reaction. For example, consider fixing \(v_x\) and varying \(v_y\), starting with \(v_y << v_x\), which corresponds to the Mg\(^+\) ions along the y-axis being much further apart than the Mg\(^+\) ions along the x-axis. This will cause both the singlet and triple states to be aligned along the x-axis. Then, deform the pyrophosphate enzyme by bringing the two ions along the y-axis closer, which will increase \(v_y\), and keep deforming the enzyme until \(v_y >> v_x\). This will cause the singlet wavefunction to rotate and align with the y-axis. However, as the triplet wavefunction cannot rotate, it will remain stuck along the x-axis and be unable to participate in the chemical reaction. Therefore, the nuclear spins of the phosphorous ions in the two Pi ions released from the pyrophosphatase will be in an entangled singlet state, as the triplet state cannot participate in the reaction.

### 4.1 Posner Molecule Entanglement

If an entangled pair of Pi ions bind to Ca\(^{+2}\) in the extracellular fluid, they can form Posner molecules. These Posner molecules will also have entangled spins. Additionally, entanglement between Posner molecules can influence the likelihood of chemical reactions, such as two Posner molecules binding to each other, occurring.

As stated above, Posner molecules contain eight calcium atoms on the corners of a cube, a ninth calcium ion at the center of the cube, and one Pi ion on each face of the cube. Therefore, it contains one threefold symmetry axis along a cube diagonal.

The spins of each phosphorous atom can be labelled by the total spin, which is an integer between 0 and 3, and a pseudo-spin, \(\sigma = 0, \pm 1\), which encodes how the state transforms under a threefold rotation.

\[
|\sigma\rangle \longrightarrow \omega^\sigma |\sigma\rangle, \quad \omega = e^{\frac{2i\pi}{3}}
\]
As both the calcium and oxygen atoms have spin 0, the full quantum state of the Posner molecule can be represented as

\[ \Psi_{P_{\text{os}}} = \sum_{\sigma} c_{\sigma} |\psi_{\sigma}(\phi)\rangle |\sigma\rangle \]  

(15)

where \( |\psi_{\sigma}(\phi)\rangle \) represents the angle of rotation about the threefold symmetry axis, the possible states of \(|\sigma\rangle\) and \(||\psi_{\sigma}\rangle\) are orthonormal, and \( \sum_{\sigma} |c_{\sigma}|^2 = 1 \). Due to the symmetry of the Posner molecule, \( \Psi_{P_{\text{os}}} \) is invariant under an 120° rotation that interchanges the position and spin of two phosphorous atoms. Therefore,

\[ |\psi_{\sigma} \left( \phi + \frac{2\pi}{3} \right) \rangle = \omega_{\sigma} |\psi_{\sigma}\rangle \]  

(16)

The combined state of two Posner molecules, \( \alpha \) and \( \alpha' \), can be represented by

\[ |\Psi_{\alpha,\alpha'}\rangle = \sum_{\sigma,\sigma'} C_{\sigma,\sigma'}^{\alpha,\alpha'} |\psi_{\sigma}^\alpha\rangle |\psi_{\sigma'}^{\alpha'}\rangle |\sigma\sigma\rangle_{\alpha,\alpha'} \]  

(17)

where \( |\psi_{\sigma}^\alpha\rangle \), \( |\psi_{\sigma'}^{\alpha'}\rangle \) represent the normalized orbital wavefunctions and \( |\sigma\sigma\rangle_{\alpha,\alpha'} \) is a spin state that encodes the possible entanglement between the two molecules. Under a 120° rotation, the spin state will be multiplied by \( \omega_{\sigma} \) and \( \omega_{\sigma'} \) while the orbital wavefunctions will be multiplied by \( \overline{\omega_{\sigma}} \) and \( \overline{\omega_{\sigma'}} \). The coefficient of each term, \( C_{\sigma,\sigma'}^{\alpha,\alpha'} \), is a 3x3 complex matrix that satisfies \( \sum_{\sigma,\sigma'} |C_{\sigma,\sigma'}^{\alpha,\alpha'}|^2 = 1 \) and encodes entanglement between the pseudo-spin and rotational states of the two molecules.

Figure 3: A pair of Posner molecules with anti-parallel symmetry axes. The former symmetry axis is oriented into the page, while the latter is oriented out of the page. \( \phi \) and \( \phi' \) represent the angles of rotation about each molecule’s respective symmetry axis.

If two Posner molecules with anti-parallel symmetry axes approach each other, they can bind and release 1 eV of energy. This chemical reaction can be described in terms of the angles \( \phi, \phi' \), which represent each molecule’s rotations.
about its respective symmetry axis. When the Posner molecules bind, $\phi = \phi' = \theta$, and the rotations stop. $\theta$ can be described by the following wavefunction

$$\chi_{\sigma\sigma'}(\theta) = \psi_\sigma^\alpha(\theta)\psi_{\sigma'}^\alpha(\theta)$$  \hspace{1cm} (18)

where

$$\chi_{\sigma\sigma'}\left(\theta + \frac{2\pi}{3}\right) = \omega_{\sigma + \sigma'}\chi(\theta)$$  \hspace{1cm} (19)

$\chi$ will also satisfy the time-independent Schrödinger equation with the following Hamiltonian

$$H = \frac{-\hbar^2}{2l_{\text{pair}}} \frac{\partial^2 \chi}{\partial \theta^2} + V(\dot{\theta})$$  \hspace{1cm} (20)

Due to the symmetry of the Posner molecules

$$V \left(\theta + \frac{\pi}{3}\right) = V(\theta)$$  \hspace{1cm} (21)

Chemical bonding of the two molecules can be modelled by the bound states of a delta-function potential

$$V = -V_0 \sum_{n=1}^{6} \delta \left(\theta - \frac{n\pi}{3}\right)$$  \hspace{1cm} (22)

Bound state solutions will only exist when $\sigma + \sigma' = 0$. Therefore, the chemical binding of two Posner molecules will induce a projective measurement of the initial state onto a state with zero pseudo-spin and release 1 eV of energy. The probability of the two molecules binding is

$$\sum_{\sigma,\sigma'} |C_{\sigma,a\sigma',a'}|^2 \delta_{\sigma + \sigma' = 0}$$  \hspace{1cm} (23)

Consider two pairs of entangled Posner molecules, $|\Psi_{aa'}\rangle \otimes |\Psi_{bb'}\rangle$. Define the variable $r$, which equals 1 if the pair $\{a,b\}$ binds and 0 if the pair doesn’t bind, and the variable $\{r'\}$ that encodes the same information for the pair $\{a',b'\}$. The probability of both pairs binding is

$$P_{rr'} = \sum_{\sigma,a,a',\sigma,b,b'} |C_{\sigma,a\sigma',a'}|^2 |C_{\sigma,b\sigma',b'}|^2 g_r(\sigma_a,\sigma_b)g_{r'}(\sigma_{a'},\sigma_{b'})$$  \hspace{1cm} (24)

$$g_1(\sigma,\sigma') = \delta_{\sigma + \sigma' = 0}, g_0(\sigma,\sigma') = 1 - g_1$$  \hspace{1cm} (25)

The degree of entanglement between the two reactions can be measured by $\epsilon = [\delta r \delta r']$, where

$$\delta r = r - [r], \delta r' = r' - [r']$$  \hspace{1cm} (26)

and all values in square brackets are defined as
\[ |f| = \sum_{r,r'} P_{r,r'} f_{r,r'} \]  

(27)

If \( \epsilon = 0 \), the wavefunctions will take on a product form, indicating no entanglement between the pairs of Posner molecules. If \( \epsilon > 0 \), the two reactions are correlated, and if \( \epsilon < 0 \), the two reactions are anti-correlated. In general, \( \epsilon \neq 0 \) for a generic entangled pair of Posner molecules, indicating that chemical bonding between the molecules has also become entangled, regardless of the distance between them. Therefore, large groups of entangled Posner molecules can induce non-locally correlated binding reactions, creating a powerful setting for quantum processing to occur.

5 Quantum Neural Processing

Even if the Posner molecules remain coherent in aqueous environments like the brain, they still need to be able to influence neuronal signalling to have an impact on cognition.

The majority of neurons communicate through chemical synapses. In the pre-synaptic neuron, neurotransmitters are transported into synaptic vesicles, which will release their contents upon reaching a threshold calcium concentration. The neurotransmitter will then diffuse across the synaptic cleft into the post-synaptic neuron, while the vesicle is recovered from the membrane.

![Figure 4: A diagram of a synapse. At high enough concentrations of calcium, synaptic vesicles in the pre-synaptic neuron will release their contents into the synaptic cleft. These neurotransmitters will diffuse across the cleft to receptors on the post-synaptic neuron. [5]](image)

Neurotransmitters are transported into synaptic vesicles through transport proteins on the vesicular membrane. For example, the vesicular transmembrane protein VGLUT uses a proton gradient to transport glutamate and a sodium (\( Na^+ \)) gradient to transport phosphate into synaptic vesicles. When the vesicles are retrieved from the pre-synaptic membrane after releasing their contents, they can engulf extracellular fluid, which has a high \( Na^+ \) concentration, and take
in Posner molecules. Once the vesicle is inside the pre-synaptic glutamateric neuron, it will grow more acidic due to the proton pumps on its membrane, and cause the Posner molecules to break down, releasing calcium and phosphate ions into the vesicle. Additionally, as the vesicle contains sodium-rich extracellular fluid, the phosphate ions can exit the vesicle and bind with calcium ions to form more Posner molecules. Furthermore, if two of these pre-synaptic Posner molecules bind, they are more likely to be broken down via hydrolysis, and release up to 18 $Ca^{+2}$ ions. This will allow the pre-synaptic neuron to remain above the the calcium concentration for longer periods of time, allowing for more synaptic vesicles to release their contents. Glutamate release causes the post-synaptic neuron to become more excitatory, so an increased amount of glutamate release from the pre-synaptic neuron will increase the firing rate of the post-synaptic neuron.

If a pair of entangled Posner molecules are transported into different neurons, their nuclear spins will still remain entangled, regardless of the physical distance between the neurons. Entanglement between pairs of Posner molecules affects the probability of the molecules in the pair binding to other Posner molecules, and bound Posner molecules are more likely to be broken down. Uptake of entangled Posner molecules by neurons can induce nuclear spin entanglement between multiple neurons, which influences the probability of the Posner molecules in each neuron binding to each other and being broken down into calcium and phosphate ions. This will influence the signalling activity of downstream post-synaptic neurons as higher concentrations of calcium increase the amount of neurotransmitter release. Therefore, uptake of entangled Posner molecules by neurons can lead to non-local quantum correlations in glutamate release from pre-synaptic neurons and the firing rate of post-synaptic neurons.

6 Conclusion

While it may seem improbable, there does exist a possible quantum mechanical influence on human brain activity. Phosphorous nuclear spins, which become entangled during pyrophosphate hydrolysis and are protected from decoherence by the calcium and oxygen atoms in Posner molecules, can serve as a neural qubit. Posner molecules can be transported into pre-synaptic glutamateric neurons via vesicle endocytosis and broken down into calcium and phosphate ions, which will both form new Posner molecules in the pre-synaptic neuron and increase its $Ca^{+2}$ concentration. The latter can lead to the release of more glutamate to the post-synaptic neuron, which will increase its firing rate. Furthermore, a pair of neurons can be entangled if each one contains half of an entangled qubit pair, leading to non-local quantum correlations between multiple neurons that influence their firing rate and likelihood of neurotransmitter release.
References


