# Quantum-classical dynamics and time irreversibility in molecular brain modeling

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### INTRODUCTION

The human brain is a remarkable system, with its intricate network of neurons and complex biochemical processes that underlie cognition, memory, and perception. As our understanding of the brain deepens, one area that has gained increasing attention is the quantum-classical dynamics within neural processes. The notion of quantum-classical interactions, particularly in terms of time irreversibility, offers a new framework for understanding how molecular mechanisms in the brain operate. In this article, we will explore the role of quantum-classical dynamics and time irreversibility in molecular brain modeling, shedding light on how these phenomena contribute to the functioning of the brain and its relationship with cognition and consciousness. In the realms of physics, the quantum and classical worlds are often seen as distinct. The classical world governs macroscopic phenomena-objects that we can directly observe and interact with, governed by deterministic laws. On the other hand, the quantum world governs microscopic phenomena, such as subatomic particles, where the principles of superposition, entanglement, and probability dominate. The behavior of quantum systems is inherently probabilistic and governed by the principles of quantum mechanics, whereas classical mechanics deals with deterministic processes. In the context of the brain, most neuroscientific models have historically relied on classical physics, which assumes that neural activity and the flow of information in the brain follow predictable patterns based on classical laws of motion and chemical interactions. However, recent research suggests that quantum phenomena might play a role in the brain's functionality. This has led to the development of quantum-classical models to understand how these two domains interact in neural systems [1].

Quantum mechanics operates at the level of individual molecules and atoms. In the brain, this could potentially influence processes such as neurotransmitter release, synaptic transmission, and ion channel activity. For example, certain proteins and enzymes that are involved in neurotransmission might exhibit quantum properties like superposition and tunneling. These quantum effects could potentially influence the behavior of the molecules in ways that classical models do not fully capture. One area where quantum effects have been observed is in the activity of ion channels. Ion channels regulate the flow of ions across neuron membranes, which is crucial for generating electrical signals and enabling communication between neurons. Some studies have suggested that these ion channels may display quantum coherence, where the particle-like behavior of ions could be influenced by quantum phenomena such as wave-particle duality or

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Word count: 1377 Tables: 03 Figures: 06 References: 05

Received: 30.01.2025, Manuscript No. ipjnn-25-15568; Editor assigned: 01.02.2025, Pre QC No. P-15568; Reviewed: 14.02.2025, QC No. Q-15568; Revised: 20.02.2025, Manuscript No. R-15568; Published: 27.02.2025

interference.

Moreover, there are hypotheses that quantum entanglement may play a role in facilitating long-range communication between distant brain regions. This would allow for rapid information exchange, even over distances that classical models would find difficult to explain. These phenomena are still under investigation, but they suggest that quantum effects could have a profound impact on brain dynamics, particularly in areas related to memory and cognition [2].

#### DESCRIPTION

The communication between neurons in the brain depends largely on neurotransmitter dynamics. These chemicals bind to receptors on adjacent neurons, triggering a cascade of biochemical events that lead to the transmission of electrical signals. It is believed that quantum effects could influence the molecular processes involved in neurotransmitter binding and receptor activation. For example, the phenomenon of quantum tunneling, where particles pass through barriers they classically should not be able to, could be involved in neurotransmitter release. In classical models, the release of neurotransmitters is a process that is governed by thermal energy, but quantum tunneling may provide an alternative pathway that allows for faster or more efficient neurotransmitter release. Additionally, quantum coherence, which is the ability of a system to maintain a stable quantum state over time, could affect how neurotransmitters interact with receptors and how information is encoded in neural networks. Quantum coherence could enhance the synchronization of neural firing patterns and facilitate more effective communication between neurons, ultimately influencing cognitive processes such as attention, learning, and memory [3].

Time irreversibility refers to the fact that certain processes cannot be reversed once they have occurred. In classical thermodynamics, this is often discussed in terms of entropy-the measure of disorder in a system. The second law of thermodynamics states that in any spontaneous process, the total entropy of a system must increase over time, meaning that the direction of time is inherently one-way. Time irreversibility is a fundamental aspect of macroscopic processes, from the cooling of a hot object to the mixing of two gases. In the brain, time irreversibility is also an important consideration. The brain operates in a dynamic, irreversible manner, particularly when it comes to the encoding and retrieval of memories. Once information is processed and stored in neural circuits, it cannot be unprocessed or "undone" in a simple manner. This irreversibility is a key feature of how the brain functions-whether in terms of synaptic plasticity, which underlies learning and memory, or in the processes of decision-making and perception.

Memory formation is inherently time-irreversible. Once information is encoded into neural circuits, it becomes part of the brain's neural architecture and cannot be simply "erased." This irreversible process is believed to involve the strengthening and weakening of synaptic connections, a process known as synaptic plasticity.

Neuroplasticity enables the brain to adapt and reorganize itself in response to new experiences, learning, and injury. In molecular terms, time irreversibility in memory formation is reflected in the changes in neurotransmitter signaling and the modification of synaptic structures. Once a memory is formed, it is encoded in the brain's synaptic weights, making it difficult to reverse or "unlearn" a memory. This reflects the classical idea of irreversible thermodynamic processes but on a biological level, driven by molecular mechanisms. Quantum effects could influence this irreversible process as well. For example, quantum coherence and entanglement might help encode and stabilize the memory in the brain's neural networks, ensuring that information remains accessible and resistant to decoherence. However, just as classical irreversible processes are governed by thermodynamic laws, quantum-classical interactions in the brain may introduce a level of unpredictability, ensuring that the brain operates in a non-reversible manner, at least at the level of neural network states and memory encoding [4].

Time irreversibility also plays a crucial role in decisionmaking processes. Once a decision is made, the choices are irreversible. Although we can re-evaluate decisions over time, the specific brain states associated with a particular decision have already passed, and they cannot be simply "undone." The processes that lead to a decision are influenced by the accumulation of past experiences, emotional responses, and cognitive biases, all of which shape our choices in an irreversible way. From a quantum-classical perspective, decision-making might involve both quantum superposition (where a decision exists in multiple states until it is observed) and classical determinism (where the final choice is determined by the brain's state). Time irreversibility in this context could stem from the brain's need to resolve these superpositions into a final, irreversible outcome. The way these quantum and classical dynamics interact could offer a deeper understanding of how the brain makes decisions and how those decisions are encoded in its neural networks [5].

### CONCLUSION

Molecular brain modeling that incorporates quantumclassical dynamics and time irreversibility represents a significant leap forward in understanding brain function. These models need to bridge the gap between quantum mechanical behavior and classical biochemical processes, offering insights into how they work together to produce cognition, memory, and consciousness. One potential approach is the development of hybrid models that combine the deterministic principles of classical neuroscience with the probabilistic nature of quantum mechanics. These models could be used to simulate neural networks that account for both the quantum states of molecules and the classical chemical signaling between neurons. By incorporating time irreversibility, these models would reflect the inherently one-way nature of processes such as memory formation and decision-making.Quantum-classical dynamics and time irreversibility offer a new and exciting lens through which to view the molecular mechanisms of the brain. By examining how quantum effects interact with classical biochemical processes, we gain a deeper understanding of how the brain operates on both a microscopic and macroscopic level. Whether in memory formation,

decision-making, or cognition, these interactions play a crucial role in shaping brain function. As we continue to explore the relationship between quantum mechanics and classical brain processes, we can look forward to new breakthroughs in neuroscience that could reshape our understanding of consciousness, cognition, and the brain itself.

# ACKNOWLEDGMENT

None.

## **CONFLICT OF INTEREST**

None.

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