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A MODEL OF QUANTUM-VON NEUMANN HYBRID CELLULAR AUTOMATA: PRINCIPLES AND SIMULATION OF QUANTUM COHERENT SUPERPOSITION AND DECOHERENCE IN CYTOSKELETAL MICROTUBULES

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Although experimental evidence suggests the influence of quantum effects in living organisms, one of the most critical problems in quantum biology is the explanation of how those effects that take place in a microscopic level can manifest in the macroscopic world of living beings. At present, quantum decoherence associated with the wave function collapse is one of the most accepted mechanisms explaining how the classical world of living beings emerges from the quantum world. Whatever the cause of wave function collapse, there exist biological systems where a biological function arises as a result of this collapse (e.g. birds navigation, plants photosynthesis, sense of smell, etc.), as well as the opposite examples (e.g. release of energy from ATP molecules at actomyosin muscle) where a biological function takes place in a quantum coherent environment. In this paper we report the modelling and simulation of quantum coherent superposition in cytoskeletal microtubules including decoherence, thus the effect of the collapse of the microtubule coherent state wave function. Our model is based on a new class of hybrid cellular automata (QvN), capable of performing as either a quantum cellular automata (QCA) or as a classical von Neumann automata (CA). These automata are able to simulate the transition or reduction from a quantum microscopic level with superposition of several quantum states, to a macroscopic level with a single stable state. Our results illustrate the significance of quantum biology explaining the emergence of some biological functions. We believe that in the future quantum biology will have a deep effect on the design of new devices, e.g. quantum hardware, in electrical engineering.

Keywords: Quantum Biology, hybrid cellular automata, wave-function collapse, emergence biological functions, coherence-decoherence modeling, cytoskeletal microtubules, human consciousness
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1 Introduction

There has been recent experimental evidence suggesting the existence of quantum phenomenon effects on living organisms [1]. For instance, birds, insects and other animals appear to use quantum coherent entanglement navigation by sensing Earth's magnetic field; plants use a form of quantum coherent superposition to find the most efficient pathway to direct energy through their photosynthetic reaction centre in the form of coherent excitons; quantum tunnelling is used by some enzymes - the molecules responsible for metabolic reactions in cells - to accelerate chemical reactions; or the sense of smell, which involves electron tunnelling between the odour molecule and a receptor in the nose. Bandyopadhyay and his group have found warm temperature quantum resonances in microtubules [2, 3]. All these examples of quantum effects in biological systems at warm temperatures have led to a new field of quantum biology which studies the role of quantum physics in biology.

One of the most critical problems in quantum biology is the explanation of how quantum effects that take place in a microscopic world can give rise to the macroscopic world of living beings. According to [4], quantum decoherence is the central mechanism by which the classical world of biological systems emerges out of a quantum system. Quantum decoherence is associated with the wave function collapse phenomenon. However, in the conventional decoherence approach of Zurek [5], decoherence doesn't necessarily cause collapse. It may just bury the quantum system in noise.

Several explanations currently attempt to justify possible mechanisms that could be responsible for wave-function collapse or reduction (**R**):

(i) **SR** (subjective reduction), where a conscious measurement or observation causes the collapse/reduction. This is the von Neumann-Wigner version of the 'Copenhagen interpretation', which puts consciousness outside science.
(ii) **OR** (objective reduction), where a reduction occurs when an objective threshold is reached.
(iii) **Orch OR** (orchestrated objective reduction), proposed by Penrose and Hameroff, where only a few (orchestrated) **OR** events result in conscious events as we know them.

In the **SR** and **Orch OR** views, consciousness is associated with reduction/collapse, but from different sides. In the **SR** interpretation, consciousness causes collapse; in **Orch OR**, consciousness is collapse.

The **Orch OR** theory is based on quantum computation in cytoskeletal microtubules in the brain's neurons. The main conjecture is that collective quantum phenomena results in coherent states in the brain. Microtubules are cylindrical polymers of subunits proteins known as tubulin, arranged in a skewed hexagonal lattice, where each tubulin subunit can exist in two or more conformational states. This model is a case of objective reduction (**OR**) where an objective threshold would cause quantum state reduction to a single state at time t, according to $t \approx \hbar / E_G$, where $\hbar = h/2\pi$ is the Dirac's form of Planck's constant h and E_G is the gravitational self-energy of the superposition mass (e.g., in a microtubule, the number of tubulins in superposition). According to the Penrose-Hameroff theory [6, 7, 8, 9], the quantumness of protein complexes such as cytoskeletal microtubules is suggested to be involved in some high level human brain capabilities opening, for instance, the possibility to understand human consciousness. According to this theory, consciousness would be a mind

'discrete experience', associated with both a gravitational **OR** process and the particular states of an organized multiparticle structure, i.e. microtubules within the neurons of the brain.

In the Penrose-Hameroff approach, decoherence is replaced by **OR** (without Orch), which means that, at the microscopic level, a superposition of several different possible eigenstates is reduced to the single state that can be observed in the macroscopic world. No matter how the wave function collapses, the aforementioned theory of mind is an example that illustrates how wave collapse is somehow related to the performance of a biological function. However, some examples illustrate the opposite view, when a biological function emerges in a quantum coherent environment [10, 11]. In such cases, some factors could be preventing decoherence and wave collapse, and allowing the maintenance of a quantum coherent environment (sustained in the brain for about 500 ms according to Hameroff and Penrose estimations) where the biological function can arise [12]. For instance, protein entanglement inside non-polar hydrophobic pockets may be extended in time as a protection from the environment; quantum superposition can be preserved with the help of a quantum error correction loophole, as has been demonstrated in a quantum computing experiment with alanine amino-acid [4]. Other examples that support this view include biological systems quasi-isolated from the decohering environment, e.g. the slow release of energy from ATP molecules at actomyosin muscle contraction; and biological systems strongly coupled to their environment resulting in the Zeno effect, which enables biological functions related with quantum coherent phenomena such as superposition and entanglement. According to Fröhlich quantum states may also be pumped by heat and energy, as in a laser [13, 14, 15]. In the realm of living beings, 'quantum coherence' typically involves multiple particles (protein subunits, excitons, electron cloud dipoles/London forces, spin states, etc.) collectively sharing a quantum state that shows space-temporal organization governed by a macroscopic wave-function. In biomolecular complexes, coherence means that the particles may exist simultaneously in a superposition of several quantum states with varying probabilities. In agreement with Davies [10, 11], quantum superposition allow the system to explore many alternative pathways simultaneously, in a manner similar to the quantum version of a search algorithm. Two good examples of these multiparticle systems showing quantum coherence are pigment-protein complexes in photosynthesis [1, 4] and microtubules [6, 7, 8, 9] in the cytoskeleton. It is interesting to note that quantum coherence in both systems shares some common elements:

- First, in microtubules, tubulin subunits tessellate a cylindrical surface, while in photosynthesis chloroplast organelles exhibit a dense packing of pigment chromophores, both made of non-polar (but polarizable) electron cloud resonance ring structures.
- Second, since both tubulin and excitons can be found in at least two states, they can explore multiple options. According to Hameroff and Penrose [6, 7, 8, 9], such exploration in microtubules could be related to high level capabilities (e.g. consciousness) in the human brain, whereas exploration in photosynthesis makes it possible to select the most efficient path to the reaction centre.
- Third, whereas some human brain faculties, i.e. consciousness, has been surmised to be related to the collapse of the wave function, in photosynthesis the collapse of the wave function occurs only after the system decides which is the most efficient pathway. In consequence, in biological systems the collapse of the wave function could just mean

that a system has found one of the best solutions for the performance of a biological function.

The cellular automata approach seems to be a useful modelling framework to study the transition from microphysics to macrophysics. In the particular case of biology, many cellular automata models focus on large-scale dynamical behaviours. This happens, for instance, in developmental biology, neurobiology, population biology [16] and pattern modelling [17, 18], e.g. pigment cell pattern, tissue and tumour development, Turing patterns, etc. This means that cellular automata are used in biology [19, 20] as models with which to study the complexity of a dynamical system in a manner similar to other disciplines, such as chemistry, physics or computer science. However, cellular automata are not only able to simulate macroscopic level phenomena adequately, they can also simulate phenomena at microscopic or quantum level [21]. In fact, one of the ways to simulate a quantum computer is based on simple quantum cellular automata [22]. Therefore, if cellular automata are able to capture the essence of both levels, it should also be possible to model and simulate the transition between these two levels of reality, i.e. the transition from the quantum world to the classical world. In a quantum world, a cellular automaton exists in a superposition of basic states which evolve according to a set of transition rules, giving rise to something that resembles a system governed by the Schrödinger equation (this deterministic evolution is referred by Penrose [23] as the **U** rule). However, when an **R** (**SR**, **OR**) event occurs, the wave function collapses to one of its basic states, and in such case the cellular automaton behaves as a classical (von Neumann) automaton. Of course, after the collapse, the cellular automaton again evolves according to the **U** rule.

Despite the interest of the simulation of the wave function collapse [24], our study focuses on the evolution of a cellular automata which behaves in some stages as a classical cellular automata and in other stages like a quantum cellular automata. In our opinion, a hybrid cellular automata with the ability to update its states in both levels of reality would allow us to simulate the transition between the states of coherence and decoherence, which could provide a better understanding of quantum effects in biological systems.

In this paper we present a hybrid cellular automata named QvN, an abbreviation for Quantum von Neumann 'hybrid' automata, capable of performing either as a quantum cellular automata (QCA) or as a classical von Neumann automata (CA), simulating the transition or reduction from a quantum microscopic level with superposition of several quantum states, to a macroscopic level with a single stable state.

Independently from the possible role of quantum physics on the human mind, which does not concern us here, we are giving an example of how these automata could be used to model and simulate quantum coherence and decoherence in cytoskeletal microtubules. In other words, our automata illustrates the quantum phenomena that could occur in cytoskeletal microtubules, apart from any consideration about whether our model corroborates (or not) the Penrose-Hameroff theory.

2 QvN model

In this cellular automata we assume that each cellular automaton is occupied by a hypothetical particle, e.g. an electron, placing the particle anywhere at a distance equal to 1. The Quantum

von Neumann 'hybrid' automata is in fact a family of models QvN defined by a set of four elements $(D_C, D, f, R_{|\psi\rangle})$:

- $D_C \in \mathbb{R}$ is the dimension of the space where the particle of each cellular automaton moves being its position described by the following vector $\vec{\theta} = (\theta_1, \theta_2, \ldots, \theta_{D_C})$.
- $D \in \mathbb{R}$ is the dimension of the cellular automata, being able to define different kinds of neighborhood, e.g. hexagonal, Moore, von Neumann, etc. Neither the shape of the grid nor the specific neighborhood is explicitly included in the QvN because they are not usually formalized and are described in each simulation experiment in an informal way. Nevertheless we will use $N_{\vec{p}}$ to represent the indexes of the neighbors of each cellular automaton at position $\vec{p} = (p_1, p_2, \ldots, p_D)$.
- f is the transition function or rule $f : \left(\mathbb{R}^D\right)^{N_{\vec{p}}} \longrightarrow \mathbb{R}^D$ that describes the state of a cellular automata in *t+1* from the state of the neighbors in *t*. In the automata, the transition rules are based on probability amplitudes [25], with a strictly local neighbourhood.
- $R_{|\psi\rangle}$ is the wave collapse mechanism associated with the transition from the quantum cellular automata to a classical von Neumann automata.

3 Modelling the quantum coherent superposition and decoherence in cytoskeletal microtubules

In this paper, we illustrate the usefulness of our automata modelling quantum coherence and decoherence in cytoskeletal microtubules, but instead of using classical cellular automata [20], we have built the model with quantum cellular automata [21]. Microtubules are cylindrical polymers of subunit proteins known as tubulin (Fig. 1) arranged in a skewed hexagonal lattice. Each tubulin state is governed by quantum mechanical London forces in nonpolar hydrophobic pockets within the protein, being plausible that tubulins can exist in quantum superposition of two conformations. Tubulin subunits are assumed to contain an electron related with α or β tubulin conformational states. Hameroff and coll. [26, 27, 28] conducted several simulations of microtubules modelled as classical von Neumann cellular automata. Based on Fröhlich excitations [13, 14, 15] as a discrete clock mechanism and defining the transition rules according to electrostatic dipole London forces in internal hydrophobic pockets of tubulins, they obtained conformational pattern behaviours similar to those observed in the Game of Life, including standing waves, oscillators and gliders. In this model, the dipole-coupled conformation for each tubulin automaton was determined at each generation by the sum of the dipoles of its six surrounding neighbours:

$$f_{net} = \frac{e^2}{4\pi\varepsilon} \sum_{i=1}^{6} \frac{y_i}{r_i^3} \tag{1}$$

where f_{net} is the sum of the six neighbour dipole forces on each tubulin, e is the electron charge, ε is the average permittivity for proteins, y_i is the *ith* neighbour in the vertical offset direction and r is the absolute distance between tubulin pairs. Tubulin states at each "clock tick" are determined by net neighbour forces according to the following transition rules: a

net value greater than a given threshold ϵ will induce a α state, while negative forces of less than$-\epsilon$ will induce a β state.

To this date, the possibility that the cytoskeletal microtubules may be suitable neuron structures for quantum coherent superposition is a possibility that has been envisioned at a theoretical level supported by theoretical arguments. Whereas in the classical von Neumann model [26, 27, 28] tubulin subunits in a microtubule switch between two bit states (0/1 or α/β), in the present model simulations are conducted assuming that each tubulin subunit can also exist as a quantum superposition (quantum bit or qubit) of both states. Thus, this model is based on the assumption that each tubulin subunit contains one qubit as a result of the superposition of London force dipoles in hydrophobic pockets. We examine the effect of the collapse of the microtubule (MT) coherent state wave function, modelling a microtubule as hybrid cellular automata capable of performing as either a quantum cellular automata (QCA) or a classical von Neumann automata (CA). Our MT automata is an example of QvN automata because of its ability to undergo a transition or reduction from a quantum microscopic level with superposition of several quantum states to a macroscopic level with a single stable state. That is, when MT behaves as a quantum cellular automata and a collapse occurs then a qubit is reduced or collapsed to a bit becoming in the cellular automata model of MT studied by Hameroff [26, 27, 28] that comes to be the result of the quantum computation performed in the MT. The simulation of the wave function collapse was conducted according to different experimental protocols.

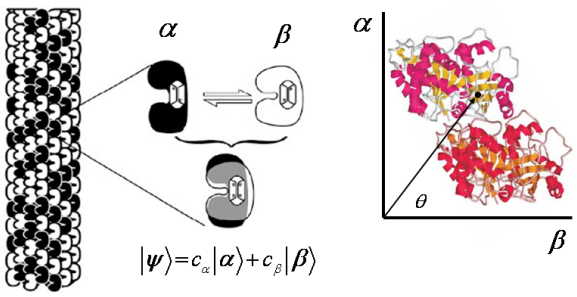

Fig. 1. (Left) Cytoskeletal microtubules are cylindrical polymers of subunit proteins known as tubulin arranged in a skewed hexagonal lattice. Each tubulin state is governed by quantum mechanical London forces in nonpolar hydrophobic pockets within the protein, being plausible that tubulins can exist in quantum superposition of two conformations. (Right) In the model each tubulin or QvN cellular automaton is assumed to contain an electron related with α or β tubulin conformational states, placing the electron anywhere on a circle with radius equal to 1 and angle θ in the range $[0,\pi/2]$.

We have modelled a MT as a 2D lattice, where each cellular automaton representing a tubulin subunit has six neighbours and exists in two possible eigenstates α or β. In agreement with Hameroff [26] each tubulin state is governed by quantum-mechanical London forces – defined by the collective positions of hundreds of electrons and summarized in the model as one electron in non-polar hydrophobic regions within proteins. The two tubulin states α and β are a consequence of a single quantum event, in particular the electron localization within a central hydrophobic pocket. The fact that tubulin states are coupled to a global protein conformation has allowed us to define a qubit as a linear combination of the two $|\alpha\rangle$ and $|\beta\rangle$

conformational eigenstates:

$$|\psi\rangle = c_\alpha |\alpha\rangle + c_\beta |\beta\rangle \tag{2}$$

where c_α and c_β are probability amplitudes. We assume that MTs modelled as quantum cellular automata are governed by quantum forces, therefore tubulin subunits can exist in the quantum superposition of both conformations, but collapse into α or β state when some reduction mechanism **R**, **SR**, **OR**, **Orch OR**, occurs. In contrast, MTs modelled as cellular automata may appear in one classical α or β state as the result of the wave function collapse of a quantum coherent state in the MT. Independently of the underlying reduction mechanism which causes wave function collapse, an interesting problem is the study of quantum evolution in a microscopic system. Evolution is defined according to [29] as a series of collapses of the wave function, i.e., which explains the microscopic quantum evolution of a MT in terms of classical macroscopic dynamical systems:

$$\psi(t + \delta t) \approx \psi(t) + \frac{\delta\psi(t)}{\delta t}\,\delta t \tag{3}$$

Accordingly, we modelled a microtubule as a QvN lattice with $D_C = 2$ and $D = 2$ dimensions, modelling each tubulin subunit as a qubit automaton occupying one lattice cell. As previously described, each cellular automaton is assumed to contain an electron related with α or β tubulin conformational states, placing the electron anywhere on a circle with radius equal to 1 and angle θ in the range $[0, \frac{\pi}{2}]$. The angle θ is represented in each cell by means of two components in the usual way (Fig. 1). Let us call these components respectively x and y. Simulation experiments were conducted setting the following parameter values: number of states (eigenstates) in each automaton (N=2), the lattice dimensions (mxn=60x59) and the seed for the random number generator (w). Different simulation experiments were performed for different initial conditions, being the initial conditions the proportion at t=0 of tubulin automata in the α eigenstate (Z_α). The Z_α value was set in the range [45, 55].

Using the nomenclature introduce by Penrose the **U** procedure, thus the deterministic evolution of the quantum system, was simulated as follows. The system is always initiated in a collapsed state, independently of the chosen mechanisms responsible of its collapse. The transition rule f for any given cell is computed by the QvN automata according to quantum amplitudes [25] by means of the following expression:

$$M_{\vec{p}}(t+1) = \sqrt{\frac{\sum_{k \in N_{\vec{p}}} M_{\vec{p}}(t)}{N_{\vec{p}}}} \tag{4}$$

The transition rule (4) computes the new states of x and y components, where $\vec{p} = (i, j)$ represents the indices used to locate each cellular automaton, thus the tubulin subunit or the qubit, in the lattice modeling the microtubule. In the rule $M_{\vec{p}}$ represents the x or y component of the cellular automaton at position $\vec{p}$ in the microtubule lattice. Finally, $N_{\vec{p}}$ represents in the MT the tubulin hexagonal neighborhood. Given a central tubulin subunit C or qubit (i, j), its 6 surrounding neighbors are the tubulin subunits or qubit automata located at cell positions $N(i, j+1)$, NE, SE, $S(i, j-1)$, SW and NW(Fig. 1). So, in our model $N_{\vec{p}} = 7$.

The simulation of quantum superposition was conducted as follows. We assume in the model that superposition of quantum states is restricted to a finite number of combinational states (seven, in our case, from $k = 0$ or β eigenstate to $k = 6$ or α eigenstate):

$$\sum_{k=0}^{6} \psi(k) |k\rangle \tag{5}$$

where each value of k is represented by a different color in the simulation experiments, that is selected based on a color gradient or ramp method. After a tubulin subunit or cellular automaton state is updated to $M_{\vec{p}}(t+1)$ state then the new combinational state $k(t+1)$ is selected according to the next expression:

$$S(t+1) = \arctan\left(\frac{M_{\vec{p}}^{x}(t+1)}{M_{\vec{p}}^{y}(t+1)}\right) \tag{6}$$

where $M_{\vec{p}}^{x}$ and $M_{\vec{p}}^{y}$ represent the x and y component of the cellular automaton at position $\vec{p}$ in the microtubule lattice. Afterwards, $k(t+1)$ is computed according to a color gradient as explained in Fig. 4.

In addition to quantum superposition property, one of the most relevant features of the QvN automata is its ability to collapse. Collapse has been defined as the operation by which each tubulin subunit, cellular automaton or qubit is reduced to a one single α or β conformational state. In our case, collapse is simulated according to a predefined collapse threshold $\theta_{|\psi\rangle}$. No matter the kind of collapse protocol $R_{|\psi\rangle}$ that is used, when the tubulin subunit or cellular automaton located at $\vec{p}$ must collapse, its next state $M_{\vec{p}}(t+1)$ is computed as follows:

$$U(t) = \arcsin\left(\sqrt{\frac{\sum_{k\in N_{\vec{p}}} M_{\vec{p}}^{x}(t)}{N_{\vec{p}}}}\right) \tag{7}$$

$$M_{\vec{p}}(t+1) = \begin{cases} \alpha, & if\ U(t) < \theta_{|\psi\rangle} \\ \beta, & if\ U(t) \geq \theta_{|\psi\rangle} \end{cases} \tag{8}$$

Note that when a collapse occurs in the microtubule, then the angle θ in each tubulin subunit, cellular automaton or qubit would be equal to 0 radians (β eigenstate) or $\pi/2$ radians (α eigenstate). We have considered two kinds of collapse protocols $R_{|\psi\rangle}$: periodic and random. In the first one, a tubulin subunit or cellular automaton collapses after a given number of generations, whereas in the second protocol the collapse is randomly decided after each generation of the automaton. Periodic collapses have been simulated every 5, 10 and 15 generations in the QvN cellular automata. Periodic and random collapses were simulated setting up a collapse threshold $\theta_{|\psi\rangle}$ equal to 0.5.

The QvN simulator has been implemented with *LabVIEW 2011*. We have followed an event driven design with these basic events:

- *Initialization.*- In this step is set up the initial α or β conformational states of the cellular automata.
- *State updating.*- Compute next generation, obtaining the *t+1* quantum superposition configuration from the current t configuration.

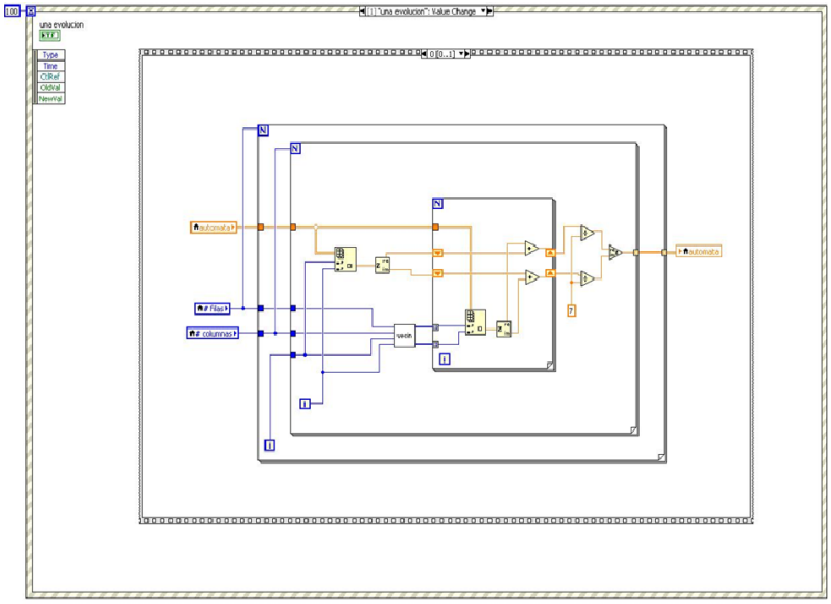

Fig. 2. LabVIEW graphical block diagram of QvN cellular automata modelling a cytoskeletal microtubule.

- *Collapse*.- In this step occurs the collapse of the current quantum superposition configuration.
- *Cellular automata pattern plotting*.- The current quantum superposition or collapsed configuration is draw using different graphical LabVIEW components.

Fig. 2 shows one of the screenshots of the LabVIEW diagrams of these basic events.

4 Results

Fig. 3 shows a plot of the 'activity' of one MT automata, measured by the Hamming distance H (the number of states which differ between two cellular automata configurations at times t and t-1) versus t. Under periodic collapse protocol (Fig. 3 (a), (b), (c)) MT automata activity decreases according to an exponential law:

$$H = \exp\left(\frac{a+b}{t}\right) \tag{9}$$

We found that a parameter depends on Z_α, thus the rate of tubulin automata at $t = 0$ in α state whereas b is influenced by the collapse generation time. In our model, H oscillates between a maximum and minimum values. Given any plausible mechanism responsible for the wave collapse, the maxima values of H represent decoherence after collapse, reducing tubulin subunits to α or β conformational states. Furthermore, in Fig. 3 the line connecting a maximum H value (this point is excluded) with another minimum H (this point is included) represents the coherent state of tubulins during quantum superposition.

Using a periodic collapse protocol we simulated the quantum phenomenon that is supposed to occur in cytoskeletal microtubules and in which rely the **Orch OR** model of human mind

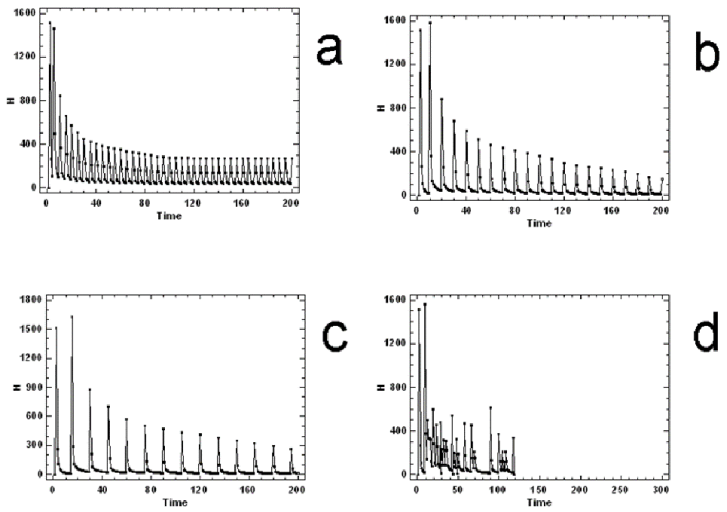

Fig. 3. MT automata activity measured by the Hamming distance H under (a, b, c) periodic collapse protocol and (d) when collapse occurs at random after each generation time.

proposed by Hameroff and Penrose [6, 7, 8, 9]. In Fig. 4 we show a microtubule automata sequence simulation in which classical von Neumann computing (times t_1, t_4, t_5 and t_8) leads to emergence of quantum coherent superposition (times t_2, t_3, t_6 and t_7). According to Hameroff and Penrose some high level brain faculties, e.g. consciousness, occur in the transitions from quantum steps to classical ones, for instance in step t_7 to t_8 transition.

Fig. 3 (d) shows a plot of the 'activity' of an MT automata - H versus time t – when collapse occurs at random after each generation time. The experiments were conducted under different collapse probabilities (0.05, 0.25, 0.5, 0.75 and 0.95).

Studying the microtubule automata sequence we observed two main MT automata patterns. Fig. 5 (a) depicts clusters of tubulins in quantum coherent superposition, resembling the 'resonance patterns' described by Hameroff and Penrose [6, 7, 8, 9]. These clusters also have a strong resemblance to isothermal lines associated to the solution of the heat Laplace equation simulated with CelLab [30]. In the biological realm, the emergence of these clusters could be explained accordingly with coherent Fröhlich excitations theory [13, 14, 15] which states that proteins are coherently synchronised by the oscillations of dipoles in the electron clouds of amino acids. In the particular case of the microtubules, Hameroff and Penrose [6, 7, 8, 9] proposed that coherence among tubulins could be achieved by thermal and biochemical energies, perhaps in the manner introduced by Fröhlich [31]. In our simulation experiments, the activity of the MT automata oscillates and decreases with time, thus in a damped fashion which from a biological point of view could be understood as a loss of energy. Note how in the simulations the MT is pumped to a higher activity level after each collapse. In consequence, there would be a shrinking of the quantum computational capability of the microtubules [32]. When in the MT automata is going on the tubulin state updating there is a greater activity than that at later stages. For this reason, we have defined MT 'Life Expectancy' as the number of iterations required to reach a constant amplitude of distance H (Fig. 3(a)). We have also found that life expectancy in microtubules is related to Z_α value.

Once a collapse occurs simulations show decohered microtubules with tubulin automata

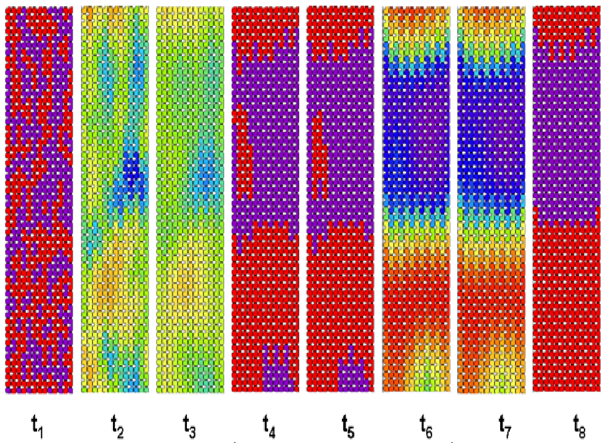

Fig. 4. Quantum coherent superposition (times t_2, t_3, t_6 and t_7) and decoherence (times t_1, t_4, t_5 and t_8) simulation in cytoskeletal microtubules (for a detailed explanation see text and [6, 7, 8, 9]) conducted with LabVIEW. Tubulin subunits ("red" represents 1 or α state, "purple" corresponds to 0 or β state) or qubit superposition states were represented according to the following color gradient or ramp: (i) If $S(t+1)$=0 (or β state) then $k(t+1)$ is 'purple' (rgb value (142, 0, 200). (ii) Color gradient is split in five regular intervals of 15 degrees. Interval $S(t+1)$ values are assigned to the colors 'dark blue' (rgb value (17, 0, 255)), 'light blue' (rgb value (42, 203, 255)), 'green' (rgb value (157, 247, 9)), 'yellow' (rgb value (255, 252, 89)) and 'orange' (rgb value (255, 174, 18)).

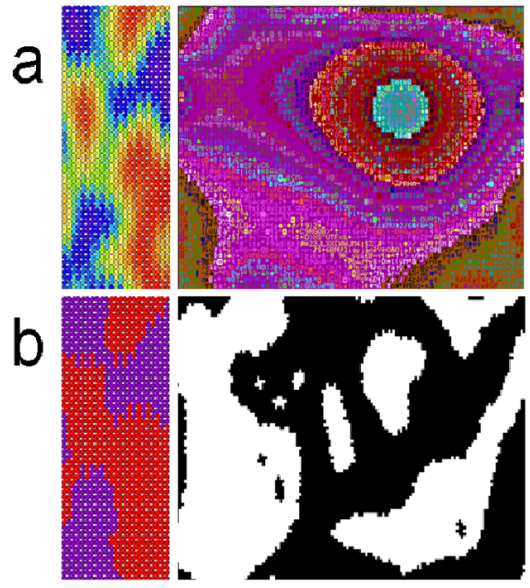

Fig. 5. (a) Clusters of tubulins in quantum coherent superposition resembling 'resonance patterns' (see Penrose-Hameroff **Orch OR** theory [6, 7, 8, 9]) and also bearing a resemblance to isothermal lines related with the solution of the heat Laplace equation. (b) Decohered microtubules with tubulin automata configurations resembling Vote cellular automata patterns.

configurations (Fig. 5(b)) resembling Vote [33] cellular automata patterns, the simplest kind of one-bit and totalistic cellular automata related to the Game of Life. In Vote, automata states are updated according to a voting rule, also known as "majority", leading to a cellular automata dynamics that bears a likeness to surface tension and to the process of metal annealing. Note that once a MT is decohered, it behaves like a classical cellular automata [26, 27, 28]. According to [10, 11, 34] we should conclude that a loss of coherence in MT could be related to the realization of a biological or physiological function. In the case of microtubules several theoretical values have been calculated as MT decoherence times, ranging from 10^{-13} s [35] to 10^{-4} or 10^{-5} s [36]. However, [4] believe that in microtubules decoherence occurs too fast to make it relevant on physiological time scales.

5 Discussion

Our simulations with QvN automata show that they are useful for the study of quantum phenomena in biological systems. The simulation of some aspects of quantum mechanics, such as superposition and decoherence, using cellular automata, would open the possibility to simulate the organization of energy transfer networks in photosynthesis, magneto-reception in birds, biochemical sensing of molecular vibrations in olfaction [1], or perhaps a possible role of quantum physics in the human mind [4].

Despite the importance of these issues, there is currently a dearth of research on building a framework for modelling and simulation of quantum phenomena in biology. There are a few examples of cellular automata that simulate natural phenomena by considering simultaneously their microscopic and macroscopic levels, which perform a simulation by connecting the processes taking place at two different levels of observation. However, in these examples the simulated microscopic level is not a quantum level. For instance:

- Weimar [37] introduced a modeling framework that couples two different types of cellular automata, a probabilistic one, simulating particles at a local level, and a second type that simulates partial differential equations at a global level. His approach is illustrated with a catalytic reaction on a surface.
- Another example is CANv2, a cellular automaton introduced by Calidonna et al. [38], which simulates a system by considering simultaneously its micro and macro-dynamics by means of a network where global behavior and local interactions can coexist. This system has been used to simulate superconductive devices and forest fires.

Boussinot's approach [39], inspired by Penrose's books, is more similar to our work. It uses a cellular automata that simulates particles embedded in a reactive environment which feature some aspects of quantum mechanics, i.e. self-interference, superposition and entanglement, including the collapse or reduction (**R**) of the system. The differences between our cellular automata and Boussinot's automata are as follows:

- In Boussinot's automata, reduction is simulated by means of detectors: special cells that react when a superposition of states reaches them. When this happens, the superposition disappears and a new particle is created in a basic state. In our QvN cellular automata, we have implemented two alternative types of collapse protocols. In the first, the automaton collapses after a given number of generations; in the second, the collapse is randomly decided after each generation of the automaton.

- The mode of collapse, or **R** procedure, is different in both models. In Boussinot's automata, the state of the particle created after the collapse is randomly chosen among the basic states making up the superposition, whereas in our automata that state is selected according to a threshold.

As in other quantum cellular automata, the **U** procedure denotes the discretized evolution of complex wave functions. In our QvN automata, we generate a discrete wave model that replaces deterministic transitions with quantum amplitudes. While other models, such as Boussinot's automata, define automata rules where the future state is given by the set of states of the neighborhood, in our cellular automata the future state of each cell follows Watrous's definition [25] of collected quantum amplitudes. Perhaps for this reason, the patterns obtained in our simulations at the quantum level (waves, ripples, etc.) bear a resemblance with those obtained by [40] with one-dimensional cellular automata governed by quantum mechanical rules. However, the simulation of a 'wave function' is not new. For instance, [41] using a cellular automaton called CAPOW, observed several wave patterns by seeding the wave with a spike, Fourier sum and random noise. Furthermore, in our model as well as the **Orch OR** model of human mind introduced by Penrose-Hameroff [6, 7, 8, 9] quantum information processing is the result of electrostatic dipole London forces in the internal hydrophobic pockets of proteins. However, Craddock and Tuszynski [42] have demonstrated the possibility of information processing at quantum level in microtubules based on excitons and phonons coupling within MTs.

One of the absent phenomena in our cellular automata is entanglement. In fact, entanglement is a non-local feature that makes a quantum cellular automata distinct from its classical counterpart. An interesting experiment would simulate entanglement within a microtubule and between microtubules connected together by MAPs proteins forming part of the same network in the cytoskeleton. Brennen and Williams [43] studied entanglement dynamics in 1D quantum cellular automata. However, in their experiments the entanglement was limited to local neighborhoods and not at large scale.

Recently, D'Ariano [44] suggested that QCA framework is very natural and promising for quantum gravity simulation. That this idea is possible is shown by the fact that quantum gravity was simulated with the help of Monte Carlo method [45] and more recently it has been simulated on a simple laptop computer also using the traditional method of Monte Carlo. In fact, [46] were able to address the simulation of quantum gravity based on a Kauffman cellular automaton. Therefore it would be feasible the simulation of the **Orch OR** reduction model with a cellular automata similar to that proposed in this paper. Apart from the role that cytoskeletal microtubules inside neurons may or may not play in consciousness, we believe that experiments of this kind with QvN automata may be of great significance in biology, helping to understand the role of the collapse of the wave function in the emergence of biological functions. Interestingly, while decoherence can be associated with the emergence of a biological function, it is one of the main difficulties in implementing quantum algorithms in physical systems as a result of the interactions of the qubits with environment. Thus, while the loss of quantum information seems useful sustaining life it is a threat to the implementation of quantum computation. Consequently, the modelling and simulation of decoherence is a relevant research topic that affects different fields of knowledge. Using classical numerical methods has been possible to solve integro-differential equations, e.g. for the case of 2P-1S transition of

hydrogen [47], and consequently successfully achieve the simulation of decoherence. However such approach requires a very small time step in order to get a reliable precision. Under such conditions conducting a simulation experiment for larger times represents a serious problem, in consequence cellular automata seems an appropriate method for decoherence modelling and simulation.

As future objectives, we believe that our research could be used in the design of quantum hardware [22], providing it with quantum biology features, such as augmenting the hardware capabilities of electronic neuro-molecular networks inspired in cytoskeletal microtubules [48]. Other possible future works are the modelling of different methods of collapse and the simulation of quantum entanglement or gravity-induced quantum collapse.

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