Cell Microtubules as Cavities: Quantum Coherence and Energy Transfer?

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Abstract A model is presented for dissipationless energy transfer in cell microtubules due to quantum coherent states. The model is based on conjectured (hydrated) ferroelectric properties of microtubular arrangements. Ferroelectricity is essential in providing the necessary isolation against thermal losses in thin interior regions, full of ordered water, near the tubulin dimer walls of the microtubule. These play the role of cavity regions, which are similar to electromagnetic cavities of quantum optics. As a result, the formation of (macroscopic) quantum coherent states of electric dipoles on the tubulin dimers may occur. Some experiments, inspired by quantum optics, are suggested for the falsification of this scenario.

Keywords: microtubules, cavities, quantum coherence, energy transfer

1 Introduction

The rôle of Quantum Mechanics in Biological Matter is naively expected to be strongly suppressed, mainly due to the 'macroscopic nature' of most biological entities as well as the fact that biological matter lives in room temperature environments. These in general result in a very fast *collapse* of the pertinent wave-functions to a classical state. However, under certain circumstances it is possible to obtain the necessary isolation against thermal losses and other environmental entanglement, so that *macroscopic* quantum-mechanical coherence, extending over scales that are considerably larger than the atomic scale, may be achieved and maintained for some time, so that certain physical processes can occur. This is precisely the point of this presentation, namely we shall make an attempt to identify biological entities that can sustain quantum coherent states responsible for energy transfer without dissipation across the cell.

In particular, we shall argue that, under certain circumstances that we shall identify below, it is possible for Cell MicroTubules (MT) [1] to operate as quantum-mechanical isolated cavities, exhibiting properties analogous to those of electromagnetic cavities used in Quantum Optics [2]. The results presented here have been obtained in collaboration with D.V. Nanopoulos. In this short communication we shall only outline the main features. For details we refer the interested reader to ref. [3].

Energy transfer across the cells, without dissipation, had been first conjectured to occur in biological matter by Fröhlich [4]. The phenomenon conjectured by Fröhlich was based on his one-dimensional superconductivity model: in one dimensional electron systems with holes, the formation of solitonic structures due to electron-hole pairing results in the transfer of electric current without dissipation. In a similar manner, Fröhlich conjectured that energy in biological matter could be transferred without dissipation, if appropriate solitonic structures are formed inside the cells. This idea has lead theorists to construct various models for the energy transfer across the cell, based on the formation of kink classical solutions [5].

In the early works no specific microscopic

models had been considered [5]. However, after the identification of the MT as one of the most important structures of the cell, both functionally and structurally, a model for their dynamics has been presented in ref. [6], in which the formation of solitonic structures, and their rôle in energy transfer across the MT, is discussed in terms of classical physics. In ref. [3] we have considered the *quantum aspects* of this one-dimensional model, and argued on the consistent quantization of the soliton solutions, as well as the fact that such semiclassical solutions may emerge as a result of 'decoherence' due to environmental entanglement, according to the ideas in [7].

The basic assumption of the model used in ref. [3] was that the fundamental structures in the MT (more specifically of the brain MT) are Ising spin chains (one-space-dimensional structures). The interaction of each chain with the neighbouring chains and the surrounding water environment had been mimicked by suitable potential terms in the one-dimensional Hamiltonian. The model describing the dynamics of such one-dimensional sub-structures was the ferroelectric distortive spin chain model of ref. [6].

Ferroelecricity is an essential ingredient for the quantum-mechanical mechanism for energy transfer we discuss here. We have conjectured [8] that the ferroelectricity which might occur in MT arrangements, will be that of hydrated ferroelectrics, i.e. the ordering of the electric dipoles will be due to the interaction of the dimers with the ordered-water molecules in the interior of the microtubular cavities. The importance of ferroelectricity lies on the fact that it induces a dynamical dielectric 'constant' $\varepsilon(\omega)$ which is dependent on the frequency ω of the excitations in the medium. Below a certain frequency, such materials are characterized by almost vanishing dynamical dielectric 'constants', which in turn implies that electrostatic interactions inversely proportional to ε might be enhanced, and thus become dominant against thermal losses. In the case of microtubules, the pertinent interactions are of electric dipole type, scaling with the distance r as $1/(\varepsilon r^3)$. For ordinary water media, the dielectric constant is of order 80. If ferroelectricity occurs, however, this is diminished significantly. As a result, the electric dipoledipole interactions may overcome the thermal losses $k_B T$ at room temperatures inside an interior cylindrical region of MT bounded by the dimer walls of thickness of order of a few Angstroms [3].

Once such an isolation is provided, it is possible for these thin interior regions to act as cavities in a way similar to that of quantum optical electromagnetic cavities ¹. The latter are characterized by coherent modes of the electromagnetic radiation. In a similar spirit, one expects that such coherent cavity modes will occur in the above-mentioned thin interior regions of MT bounded by the protein dimer walls. Indeed, as we discussed in [3], these modes are provided by the interaction of the electric dipole moments of the ordered-water molecules in the interior of MT with the quantised electromagnetic radiation [10, 11]. Such coherent modes are termed *dipole quanta*.

It is the interaction of such 'cavity' modes with the electric dipole excitations of the dimers that leads to the formation of coherent (dipole) states on the tubulin dimer walls of MT. A review of how this can happen, and by what means one can test such a situation experimentally, will be the main topic of this communication.

2 Microtubules and Coherent States

Microtubules are hollow cylinders comprised of an exterior surface of cross-section diameter 25 nm (1 $nm = 10^{-9}$ meters) with 13 arrays (protofilaments) of protein dimers called tubulines [1]. The interior of the cylinder, of cross-section diameter 14 nm, contains ordered water molecules, which implies the existence of

¹Note that the role of MT as waveguides has been proposed by S. Hameroff already some time ago [9]. However, in our scenario we look for isolated regions inside the MT which play the role of cavities.

an electric dipole moment and an electric field. We stress that the *ordered water* may be different from ordinary water. The arrangement of the dimers is such that, if one ignores their size, they resemble triangular lattices on the MT surface. Each dimer consists of two hydrophobic protein pockets, and has an unpaired electron. There are two possible positions of the electron, called α and β conformations. When the electron is in the β -conformation there is a 29° distortion of the electric dipole moment as compared to the α conformation.

In standard models for the simulation of the MT dynamics [6], the 'physical' degree of freedom - relevant for the description of the energy transfer - is the projection of the electric dipole moment on the longitudinal symmetry axis (xaxis) of the MT cylinder. The 29° distortion of the β -conformation leads to a displacement u_n along the x-axis, which is thus the relevant physical degree of freedom. This way, the effective system is one-dimensional (spatial), and one has the possibility of a quantum integrable system [3].

Information processing occurs via interactions among the MT protofilament chains. The system may be considered as similar to a model of interacting Ising chains on a triangular lattice, the latter being defined on the plane stemming from filleting open and flattening the cylindrical surface of MT. Classically, the various dimers can occur in either α or β conformations. Each dimer is influenced by the neighbouring dimers resulting in the possibility of a transition. This is the basis for classical information processing, which constitutes the picture of a (classical) cellular automatum.

The quantum nature of a MT network results from the assumption that each dimer finds itself in a superposition of α and β conformations. Viewed as a two-state quantum mechanical system, the MT tubulin dimers couple to conformational changes with $10^{-9} - 10^{-11}$ sec transitions, corresponding to an angular frequency $\omega \sim \mathcal{O}(10^{10}) - \mathcal{O}(10^{12})$ Hz. In the present work we assume the upper bound of this frequency range to represent (in order of magnitude) the characteristic frequency of the dimers, viewed as a two-state quantum-mechanical system:

$$\omega_0 \sim \mathcal{O}(10^{12}) \text{ Hz} \tag{1}$$

As we shall see below, such frequency range is not unusual for biological matter.

Let u_n be the displacement field of the *n*th dimer in a MT chain. The continuous approximation proves sufficient for the study of phenomena associated with energy transfer in biological cells, and this implies that one can make the replacement

$$u_n \to u(x,t)$$
 (2)

with x a spatial coordinate along the longitudinal symmetry axis of the MT. There is a time variable t due to fluctuations of the displacements u(x) as a result of the dipole oscillations in the dimers.

The effects of the neighbouring dimers (including neighbouring chains) can be phenomenologically accounted for by an effective potential V(u). In the model of ref. [6] a double-well potential was used, leading to a classical kink solution for the u(x,t) field. More complicated interactions are allowed in the picture of ref. [3], where more generic polynomial potentials have been considered.

The effects of the surrounding water molecules can be summarised by a viscous force term that damps out the dimer oscillations,

$$F = -\gamma \partial_t u \tag{3}$$

with γ determined phenomenologically at this stage. This friction should be viewed as an environmental effect, which however does not lead to energy dissipation, as a result of the non-trivial solitonic structure of the groundstate and the non-zero constant force due to the electric field. This is a well known result, directly relevant to energy transfer in biological systems [5].

In mathematical terms the effective equation of motion for the relevant field degree of freedom u(x, t) reads:

$$u''(\xi) + \rho u'(\xi) = P(u)$$
 (4)

where $\xi = x - vt$, v is the velocity of the soliton, $\rho \propto \gamma$ [6], and P(u) is a polynomial in u, of a certain degree, stemming from the variations of the potential V(u) describing interactions among the MT chains [3]. In the mathematical literature [12] there has been a classification of solutions of equations of this form. For certain forms of the potential [3] the solutions include *kink solitons* that may be responsible for dissipation-free energy transfer in biological cells [5]:

$$u(x,t) \sim c_1 \left(tanh[c_2(x-vt)] + c_3 \right)$$
 (5)

where c_1, c_2, c_3 are constants depending on the parameters of the dimer lattice model. For the form of the potential assumed in the model of [6] there are solitons of the form $u(x,t) = c'_1 + c'_1$ $\frac{c'_2 - c'_1}{1 + e^{c'_3(c'_2 - c'_1)(x - vt)}}$, where again $c'_i, i = 1, \dots 3$ are appropriate constants.

A semiclassical quantization of such solitonic states has been considered in [3]. The result of such a quantization yields a modified soliton equation for the (quantum corrected) field $u_{a}(x,t)$ [13]

$$\partial_t^2 u_q(x,t) - \partial_x^2 u_q(x,t) + \mathcal{M}^{(1)}[u_q(x,t)] = 0 \quad (6)$$

with the notation

 $M^{(n)} = e^{\frac{1}{2}(G(x,x,t) - G_0(x,x))\frac{\partial^2}{\partial z^2}} U^{(n)}(z)|_{z = u_q(x,t)},$ and $U^{(n)} \equiv d^n U/dz^n$. The quantity U denotes the potential of the original soliton Hamiltonian, and G(x, y, t) is a bilocal field that describes quantum corrections due to the modified boson field around the soliton. The quantities $M^{(n)}$ carry information about the quantum corrections. For the kink soliton (5) the quantum corrections (6) have been calculated explicitly in ref. [13], thereby providing us with a concrete example of a large-scale quantum coherent state.

A typical propagation velocity of the kink solitons (e.g. in the model of ref. [6]) is $v~\sim~2$ m/sec, although, models with $v~\sim$ 20 m/sec have also been considered [14]. This implies that, for moderately long microtubules of length $L \sim 10^{-6}$ m, such kinks transport energy without dissipation in

$$t_F \sim 5 \times 10^{-7} \text{ sec} \tag{7}$$

As we shall see in the next section, such time scales are comparable to, or smaller in magnitude than, the decoherence time scale of the above-described coherent (solitonic) states $u_a(x,t).$ This implies the possibility that fundamental quantum mechanical phenomena may then be responsible for frictionless energy (and signal) transfer across microtubular arrangements in the cell.

3 Microtubules as Cavities

In ref. [3] we have presented a microscopic analysis of the physics underlying the interaction of the water molecules with the dimers of the MT, which is responsible for providing the friction term (3) in the effective (continuum) description. Below we review briefly the scenario. As a result of the ordered structure of the water environment in the interia of MT. there appear *collective* coherent modes, the socalled dipole quanta [10]. These arise from the interaction of the electric dipole moment of the water molecule with the quantised radiation of the electromagnetic field [11], which may be self-generated in the case of MT arrangements [14, 3]. Such coherent modes play the role of 'cavity modes' in the quantum optics terminology. These in turn interact with the dimer structures, mainly through the unpaired electrons of the dimers, leading to the formation of a quantum coherent solitonic state that may extend even over the entire MT network. As mentioned above, such states may be identified [3] with semi-classical solutions of the friction equations (4). These coherent, almost classical, states should be viewed as the result of *decoherence* of the dimer system due to its interaction/coupling with the water environment [7].

Such a dimer/water coupling can lead to a situation analogous to that of atoms interacting with coherent modes of the electromagnetic radiation in quantum optics Cavities, namely to the so-called Vacuum-Field Rabi Splitting (VFRS) effect [15]. VFRS appears in both the emission and absorption [16] spectra of atoms in interaction with a coherent mode of electromagnetic radiation in a cavity. For our purposes below we shall review the phenomenon by restricting ourselves for definiteness to the absorption spectra case.

Consider a collection of N atoms of frequency ω_0 inside an electromagnetic cavity, to which it is injected a pulse of an external field, of frequency Ω . Then, there is a doublet structure (splitting) of the absorption spectrum of the atom-cavity system with peaks at:

$$\Omega = \omega_0 - \Delta/2 \pm \frac{1}{2} (\Delta^2 + 4N\lambda^2)^{1/2} \quad (8)$$

where $\Delta = \omega_c - \omega_0$ is the detuning of the cavity mode, of frequency ω_c , compared to the atom frequency. For resonant cavities the splitting occurs with equal weights

$$\Omega = \omega_0 \pm \lambda \sqrt{N} \tag{9}$$

Notice here the enhancement of the effect for multi-atom systems N >> 1. The quantity $2\lambda\sqrt{N}$ is called the 'Rabi frequency' [15]. From the emission-spectrum theoretical analysis an estimate of λ may be inferred which involves the matrix element, \underline{d} , of atomic electric dipole between the energy states of the twolevel atom [15]:

$$\lambda = \frac{E_c \underline{d} \cdot \underline{\epsilon}}{\hbar} \tag{10}$$

where $\underline{\epsilon}$ is the cavity (radiation) mode polarisation, and

$$E_c \sim \left(\frac{2\pi\hbar\omega_c}{\varepsilon V}\right)^{1/2} \tag{11}$$

is the r.m.s. vacuum (electric) field amplitude at the centre of a cavity of volume V, and of frequency ω_c , with ε the dielectric constant of the medium inside the volume V. In atomic physics the VFRS effect has been confirmed by experiments involving beams of Rydberg atoms resonantly coupled to superconducting cavities [17].

Under the analogy between the thin cavity regions near the dimer walls of MT with the above-mentioned electromagnetic cavities, the role of atoms in this case is played by the unpaired two-state electrons of the tubulin dimers [3] oscillating with a frequency (1). To estimate the Rabi coupling between cavity modes and such dimer oscillations, one should use (10) for the MT case. The electric dipole moment d in that case may be estimated as follows: each dimer has a mobile charge [1]: $q = 18 \times 2e$, e the electron charge, and we use the fact that a typical distance for the estimate of the electric dipole moment for the 'atomic' transition between the α, β conformations is of order of the distance between the two hydrophobic dimer pockets, i.e. $\mathcal{O}(4 \text{ nm})$. This yields

$$d_{dimer} \sim 3 \times 10^{-18} \text{ Cb} \times \text{Angstrom}$$
(12)

We also took account of the fact that, as a result of the water environment, the electric charge of the dimers appears to be screened by the relative dielectric constant of the water, which in units of that of the vacuum is $\varepsilon/\varepsilon_0 \sim 80$. We note, however, that the biological environment of the unpaired electric charges in the dimer may lead to further suppression of d_{dimer} (12).

We have used some simplified models for the ordered-water molecules, which yield [3] a frequency of the coherent dipole quanta ('cavity' modes) of order:

$$\omega_c \sim 6 \times 10^{12} s^{-1} \tag{13}$$

Notably this is of the same order as the characteristic frequency of the dimers (1), implying that the dominant cavity mode and the dimer system are almost in resonance in the scenario of [3]. Note that this is a feature shared by the Atomic Physics systems in Cavities, and thus we may apply the pertinent formalism to our system. Assuming a relative dielectric constant of water w.r.t to that of vacuum ϵ_0 , $\varepsilon/\varepsilon_0 \sim 80$, one obtains from (11) for the case of MT cavities:

$$E_c \sim 10^4 \text{ V/m} \tag{14}$$

Notably, electric fields of such a magnitude can be provided by the electromagnetic interactions of the MT dimer chains, the latter viewed as giant electric dipoles [6]. This may be seen to suggest that the coherent modes ω_c , which in our scenario interact with the unpaired electric charges of the dimers and produce the kink solitons along the chains, owe their existence to the (quantised) electromagnetic interactions of the dimers themselves.

The Rabi coupling for the MT case then is estimated from (10) to be of order:

Rabi coupling for MT
$$\equiv \lambda_{MT} = \sqrt{N}\lambda_0 \sim 3 \times 10^{11} s^{-1}$$
 (15)

which is, on average, an order of magnitude smaller than the characteristic frequency of the dimers (1).

In the above analysis, it was assumed that the system of MT dimers interacts with a *single* dipole-quantum coherent mode of the ordered water and hence interactions among the dimer spins were ignored. More complicated situations, involving interactions either among the dimers or of the dimers with more than one radiation quanta, which undoubtedly occur in nature, may affect the above estimate.

The presence of such a coupling between water molecules and dimers leads to quantum coherent solitonic states of electric dipole quanta on the tubulin dimer walls. To estimate the decoherence time we remark that the main source of dissipation (environmental entanglement) comes from the imperfect walls of the cavities, which lose coherent modes and energy. The time scale, T_r , over which a cavity MT dissipates its energy, can be identified in our model with the average life-time t_L of a coherent-dipole quantum state, which has been found to be [3]: $T_r \sim t_L \sim 10^{-4}$ sec. This leads to a naive estimate of the quality factor for the MT cavities, $Q_{MT} \sim \omega_c T_r \sim \mathcal{O}(10^8)$. We note, for comparison, that high-quality cavities encountered in Rydberg atom experiments dissipate energy in time scales of $\mathcal{O}(10^{-3}) - \mathcal{O}(10^{-4})$ sec, and have Q's which are comparable to Q_{MT} above. The analysis of [3] then yields the following estimate for the collapse time of the kink coherent state of the MT dimers due

to dissipation:

$$t_{collapse} \sim \mathcal{O}(10^{-7}) - \mathcal{O}(10^{-6}) \text{ sec} \qquad (16)$$

This is larger than the time scale (7) required for energy transport across the MT by an average kink soliton in the models of [6, 14]. The result (16), then, implies that Quantum Physics may not be irrelevant as far as dissipationless energy transfer across the MT is concerned.

In view of this specific model, we are therefore in disagreement at this stage with the conclusions of [18], that only classical physics is responsible for energy and signal transfer in brain MT. Such conclusions did not take proper account of the possible isolation against environmental entanglement, which may occur inside certain regions of MT.

4 Conclusions and Outlook

In [3] we have put forward a conjecture concerning the representation of certain regions inside the MT arrangements in the cell as *isolated* high-Q(uality) *cavities*. We presented a scenario according to which the presence of the ordered water in the interior of the MT cylindrical arrangements results in the appearance of electric dipole quantum coherent modes, which couple to the unpaired electrons of the MT dimers via Rabi vacuum field couplings. The situation is analogous to the physics of Rydberg atoms in electromagnetic cavities [15]. In quantum optics, such couplings may be considered as experimental proof of the quantised nature of the electromagnetic radiation. In our case, therefore, if present, such couplings could indicate the existence of the coherent quantum modes of electric dipole quanta in the ordered water environment of MT, conjectured in ref. [10, 11], and used here.

To verify experimentally such a situation, one should first check on the ferroelectric properties of the MT arrangements, which the above analysis is crucially based on, and measure the corresponding dipole moments of the tubulin dimers. A suggestion along these lines has been put forward in ref. [8].

In addition, one should verify the aforementioned Vacuum field Rabi coupling (VFRS), λ_{MT} , between the MT dimers and the ordered water quantum coherent modes. This coupling, if present, could be tested experimentally by the same methods used to measure VFRS in atomic physics [17], i.e. by using the MT themselves as *cavity environments*, in the way described above, and considering tunable probes to excite the coupled dimerwater system. Such probes could be pulses of (monochromatic) light, for example, passing through the hollow cylinders of the MT. This would be the analogue of an external field in the atomic experiments mentioned above. The field would then resonate, not at the bare frequencies of the coherent dipole quanta or dimers, but at the *Rabi splitted* ones, leading to a double peak in the absorption spectra of the dimers [17]. By using MT of different sizes one could thus check on the characteristic \sqrt{N} enhancement of the (resonant) Rabi coupling (9) for MT systems with N dimens.

Clearly much more work needs to be carried out before even tentative conclusions are reached, concerning the nature of the MT arrangements inside the cell. Moreover, one should always bear in mind that the extrapolation of results obtained *in vitro* to *in vivo* situations may not always be feasible. However, we believe that the above theoretical ideas and experimental suggestions constitute a useful addition to the programme of understanding the dynamics of Microtubules, and the associated processes of energy and signal (stimuli) transfer across the cells.

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