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Microtubules as mechanical force sensors

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Abstract

Microtubules are polymers of tubulin subunits (dimers) arranged on a hexagonal lattice. Each tubulin dimer comprises two monomers, the α-tubulin and β-tubulin, and can be found in two states. In the first state a mobile negative charge is located into the α-tubulin monomer and in the second into the β-tubulin monomer. Each tubulin dimer is modeled as an electrical dipole coupled to its neighbors by electrostatic forces. The location of the mobile charge in each dimer depends on the location of the charges in the dimer's neighborhood. Mechanical forces that act on the microtubule affect the distances between the dimers and alter the electrostatic potential. Changes in this potential affect the mobile negative charge location in each dimer and the charge distribution in the microtubule. The net effect is that mechanical forces affect the charge distribution in microtubules. We propose to exploit this effect and use microtubules as mechanical force sensors. We model each dimer as a two-state quantum system and, following the quantum computation paradigm, we use discrete quantum random walk on the hexagonal microtubule lattice to determine the charge distribution. Different forces applied on the microtubule are modeled as different coin biases leading to different probability distributions of the quantum walker location, which are directly connected to different charge distributions. Simulation results show that there is a strong indication that microtubules can be used as mechanical force sensors and that they can also detect the force directions and magnitudes.

Keywords: Microtubules; Tubulin; Force sensors; Quantum walk; Quantum computing

1. Introduction

The cytoskeleton is a network of fibrous proteins that give the cell shape, strength and rigidity. These fibrous proteins control cellular movement by generating forces required for cell migration and control also movements within the cell (Lodish et al., 1995). Additionally, they provide the framework to which cellular organelles are attached. The cytoskeleton is composed of three fibrous protein systems: the microfilaments, the intermediate filaments and the microtubules (Wolfe, 1993).

Microtubules are polymers of tubulin subunits (dimers) arranged on a hexagonal lattice. Each tubulin dimer comprises two monomers, the α-tubulin and β-tubulin, and can be found in two states. In the first state a mobile negative charge is located into the α-tubulin monomer and in the second into the β-tubulin monomer. Each dimer is a dipole with the mobile negative charge usually localized into the α-tubulin monomer (Baker et al., 2001).

Microtubules can not only generate forces but can also sense forces, such as gravitational ones, which

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affect their formation and function (Tabony et al., 2001). Except from force generation and sensing, microtubules can propagate signals (Brown and Tuszynski, 1997), process information (Tuszynski et al., 1995) and perform elementary quantum computations (Hagan et al., 2002). Furthermore, is has been shown that the geometric curvature of microtubules may play a significant role in information processing (Clark, 1996).

Since microtubules can sense forces, transmit signals and process information the question follows naturally: can microtubules be used as mechanical force sensors? The aim of this paper is to study the feasibility of using microtubules as smart or even intelligent mechanical force sensors.

For this study, we modeled each tubulin dimer as a two-state quantum system and used a quantum computer simulator (Karafyllidis, 2005), which has been successfully tested in simulating entanglement generation and variation (Karafyllidis, 2004a), and cellular quantum architectures (Karafyllidis, 2003).

The proposed method for mechanical force sensing is to excite a tubulin dimer located near the center of the microtubule. This excitation will result in mobile charge transport from α to β-monomer, which in turn will trigger charge movements from α to β-monomers in the neighborhood and so on. The microtubule acts as a quantum cellular automaton (Karafyllidis, 2004b). Forces that act on the microtubule affect the distances between the dimers and alter the electrostatic potential. Changes in this potential affect the mobile negative charge location in each dimer and the charge distribution in the microtubule. The net effect is that mechanical forces affect the charge distribution in microtubules. The whole process is modeled as a quantum walk on the microtubule lattice (Kempe, 2003; Carneiro et al., 2005). The charge distributions can be measured using single-electron nanoelectronic gates and circuitry (Karafyllidis, 2002; Zardalidis and Karafyllidis, 2003).

Simulation results show a significant difference in charge distribution when different forces act on the microtubule. This is a very strong indication that microtubules cannot only sense mechanical forces, but can even detect the direction and magnitude of the force.

This paper is organized as follows: In Section 2 the structure of microtubules is presented. Two-dimensional quantum walks, the model of the microtubule as a lattice of two-state quantum systems (tubulin dimers) and the formulation of the quantum walk on this lattice are given in Section 3. The simulation and the simulation results are presented in Section 4 and the conclusions in Section 5.

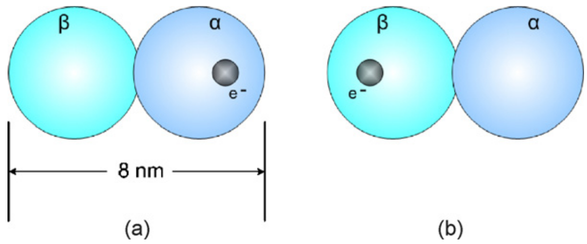

Fig. 1. Schematic representation of a tubulin dimer, with (a) the mobile negative charge in the α-monomer and (b) with the mobile negative charge in the β-monomer.

2. Tubulin and microtubules

Microtubules are hollow cylinders with an outer diameter of 25 nm and inner diameter of 15 nm. They are made of tubulin dimers arranged on a hexagonal lattice with helical symmetry. The microtubule cylinder comprises 13 protofilaments (tubulin columns). Each tubulin dimer comprises two monomers, the α-tubulin and β-tubulin, its length is 8 nm and its height is 5 nm (Tuszynski et al., 1995).

The tubulin dimer is represented by two equally sized spheres representing the α and β-monomers, as shown in Fig. 1. Each dimer contains a mobile negative charge, usually an electron, which is located either into the α (Fig. 1(a)) or the β-monomer (Fig. 1(b)).

Fig. 2 shows a part of the microtubule lattice. Fig. 2(a) shows a tubulin dimer and its six neighboring dimers. These dimers form a hexagon shown in Fig. 2(b) and (c).

The microtubule lattice is composed of hexagons like the one shown in Fig. 2(c). To model and simulate the microtubule as a mechanical force sensor we chose to use the primitive lattice cell shown in Fig. 3. This cell is formed by drawing lines to connect a given lattice site (point) to all neighboring lattice points. New lines are drawn at the midpoints and normal to these lines. The smallest area enclosed by these lines is the primitive cell (Kittel, 1976). This primitive cell is the grey area in Fig. 3 and from now on will be referred to as "microtubule cell".

Fig. 3 also shows the three lattice directions i, j and k. The angle between i and j directions is 45.6° and the angle between j and k is 58.2° (Mershin et al., 2004; Tuszynski et al., 1995). Based on the tubulin and microtubule lattice geometry, we constructed a microtubule lattice formed by microtubule cells, shown in Fig. 4. Each microtubule cell contains a tubulin dimer. This lattice will be used for the simulation of the microtubule as a mechanical force sensor.