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A theory for cell microtubule wall in external field and pseudo-spin wave excitation

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Abstract

The cytoskeleton of eukaryotic cells contains networks of protein polymers called microtubules (MTs), which provide a wide range of microskeletal and micromuscular functionalities. Evidences from a number of directions suggest that they can also serve as a medium for intracellular signal processing. For the inherent symmetry structures and the electric properties of the microtubule (MT), we treat the MT wall as a one-dimension ferroelectric system and describe the nonlinear dynamics of the dimer electric dipoles with the double-well potential, and then map the physical problems onto the pseudo-spin system. By using the random phase approximation, the effect from the external electric field has been taken into account. We have developed an expression for the Hamiltonian in the pseudo-spin system and obtained the coupled motion equations for the disturbed pseudo-spin wave, and there appears to be a transverse collective excitation with an intrinsic frequency.

Keywords: Microtubule; Double-well potential; Pseudo-spin; External electric field; Random phase approximation

1. Introduction

The cytoskeletal microtubule (MT) has recently received considerable attention from number of physicists [1–5]. By virtue of the networks of interconnected protein polymers, the interiors of biological cells are highly organized in both structure and dynamics. These networks are referred to as well known cytoskeleton. The cytoskeletons comprise various protofilaments. Among those protofilaments, Microtubules (MTs) are the very important for cellular organization and information processing. MTs are almost ubiquitous in the entire biology, especially enriched in brain tissue [4].

X-ray crystallography shows that MT is a hollow cylindrical tube about 25 nm in outer diameter and 14 nm in inner diameter [1]. The interior of the cylinder is likely to be filled with ordered water, which implies the existence of electric dipoles and electric field. The outer surface of MT is surrounded by oriented molecules of

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cytoplasmic water and enzymes. MT wall is an assembly of 13 protofilaments, each of which is a series of subunit proteins known as tubulin dimers. Measurements by electron crystallography [5] have further demonstrated the structure of the tubulin subunit. Each tubulin subunit is an 8-nm peanut-shaped dimer consisting of two nearly identical 4-nm monomers called α- and β-tubulin, respectively. There is an unbound mobile electron on each tubulin dimer, which can be localized either more toward the α-monomer or more toward the β-monomer. So according to the localization of the mobile electron, the tubulin dimer protein has two basic states $|\alpha\rangle$ and $|\beta\rangle$. Induced by the GTP$\rightarrow$GDP hydrolysis, there is a conformational change, from the $|\alpha\rangle$ to the $|\beta\rangle$ state, depending on the relocalization of the unbound mobile electron in its hydrophobic protein pocket. Therefore, MTs are oriented assemblies of electric dipoles and can be identified as electret substances with ferroelectric properties [6–8].

Some models for MT dynamics have been presented [6–10]. For tubulin dimer dipoles in protofilament of a MT, Sataric et al. have taken the well-known double-well potential model to describe its nonlinear dynamic behavior [8]. This model is very successful in describing bistable molecular systems [11], dipolar excitations in ferroelectrics [12] and other relevant fields. In this paper, we study the nonlinear dynamic behavior of dimer-electric dipoles in the protofilament, and utilize the double-well potential to represent each $\alpha\beta$-dimer. Furthermore, according to the quantum character of mobile electrons, we further take the pseudo-spin model to describe the system.

2. The physical model and the Hamiltonian of the system

We utilize the double-well potential to represent each $\alpha\beta$-tubulin dimer in one protofilament of a MT [8]. The single mobile electron on each $\alpha\beta$-tubulin dimer can be localized at the site of the α-monomer or the site of the β-monomer. Correspondently, this mobile electron can be localized in either well of this double-well potential. Under certain conditions, the electron may go from one well into the other by quantum tunneling penetration. The ground state of the electron in each potential well is a doublet state. The tunneling penetration effect may eliminate this degeneracy, and hence crucially influence the dynamic property of the system. It is possible that the electron may occupy the higher excitation states. But here, we prefer to assume that the energy differences between these excited states and the ground state are quite large compared with the splitting energy of the doublet state. And then we neglect the contributions from the excited states and consider only the doublet state. According to the quantum characters of mobile electrons and the spin wave theory developed in the solid-state physics [13] and ferroelectricity theory [14], each such double well may be represented by one pseudo-spin. The two possible orientations of the pseudo-spin, up and down, correspond to the two possible localized positions of the mobile electron, the site of α-well and the site of β-well. Using the pseudo-spin wave of the system, we can describe the distribution and the dynamic behavior of mobile electrons on the protofilament.

The Hamiltonian operator $\hat{H}$ for the system of the electrons consists of three parts, the kinetic energy of the electrons, the effective potential energy related to the double-well potential in the one-dimensional chain of tubulin dimers, and the Coulomb interaction energy between the electrons. Because the Coulomb interaction energy makes by far the greatest contribution of all the interaction energies between the electrons, the Hamiltonian operator $\hat{H}$ for the system may be divided into two parts: one part describing the one-body problem (movement) and the second part describing the two-body electron–electron Coulomb interaction. In the framework of quantum field theory [13], the explicit form of $\hat{H}$ mentioned above is as follows:

$$\hat{H} = \int \psi^{+}(x)\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{eff}}(x)\right)\psi(x)\,\mathrm{d}x + \frac{1}{2}\iint \psi^{+}(x)\psi^{+}(x')\frac{e^2}{\varepsilon|x-x'|}\psi(x')\psi(x)\,\mathrm{d}x\,\mathrm{d}x', \tag{1}$$

where $\psi^{+}(x)$ and $\psi(x)$ are particle field operators. They satisfy the Fermi commutation relations, and can be expanded in terms of Wannier functions in the form

$$\psi^{+}(x) = \sum_{i\lambda} a^{+}_{i\lambda} W^{*}_{\lambda}(x-i),$$

$$\psi(x) = \sum_{i\lambda} a_{i\lambda} W_{\lambda}(x-i). \tag{2}$$