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Dynamics of Microtubule Pseudo-Spin under the Influence of External Electric Field

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Abstract In this paper, the longitudinal polarization (order parameter) and electric susceptibility in the microtubule system have been investigated in the absence and presence of an external electric field using the mean-field approximation (MFA). We analyzed the behavior of the pseudo-spins inside the tubulin dimers by the transverse Ising approximation. We found out that in the absence of the electric field, the coupling constant of spin-spin interaction and anisotropic interaction bring the system in a ferroelectric (FE) phase while high temperatures and transverse fields bring the transition to paraelectric (PE) phase. Moreover, the presence of an external electric field increases the critical temperatures and brings the hysteresis phenomenon in the microtubule system.

Keywords Microtubule, Polarization, Transverse field, Ferroelectric phase, External electric field, Temperature

1. Introduction

The cytoskeleton is an assembly of multiple proteins connect together in order to give and maintain cell and membrane shape. In the cytoskeleton, there are three types of filament namely: actin filaments, intermediate filaments, and microtubules (MTs) [1,2]. MTs, major elements of the cytoskeleton are supposed to be the center of cellular organization and information processing. They play an important role in intracellular transport where they serve as road-rail for motors proteins, essential during cell division and cell motility [3,4]. For example, the coronavirus, hepatitis C virus, and many other viruses interact with microtubules directly or indirectly by associating with motor proteins [5] to move through the multiplication areas of the cell and facilitate replication of the virus. The perturbation of the displacement of microtubules associated with the coronavirus slows the replication of the virus [6-8].

It had been shown that MT is a long cylindrical tube about 25nm in outer diameter and 14nm in inner diameter. The interior of the cylinder is likely to be filled with ordered water, which implies the existence of electric dipoles and electric fields [9,10]. Forms by 13 protofilaments, MTs are extremely dynamic and unstable because of the dynamic behavior of its basic units call tubulin dimers that attach end to end to form a protofilament [11,12]. Each tubulin dimer consists of two elements, α tubulin negatively charged and β tubulin positively charged. This polarity difference implies that MTs are polarized structures where tubulin dimers are seen as electric dipoles [13,14]. There is an unbound mobile electron on each dimer, which can be localized to either α tubulin or β tubulin. Thus, depending on the location of the mobile electron, the tubulin dimer has two basic states as shown in Fig.1. These states are pseudo-spins where one can be spin up and another spin down depending on the mobility of electrons in the tubulin dimer [15,16]. In agreement with the behavior of ferroelectric (FE) materials to have a spontaneous electric polarization whose direction of polarization can be reversed under the action of an electric field [17-20], it has been hypothesized that MTs are oriented assemblies of electrical dipoles and can be assimilated to ferroelectric systems [21]. In ferroelectric systems, polarization is considered as the order parameter to describe the entire system. In classical electrodynamics, it is a macroscopic quantity defined as the average of the local contribution of elementary dipole moments and quantifies the transition from ferroelectric to paraelectric (PE-PE) phase [22,23]. In general, the system is usually considered in the ordered state or ferroelectric state when spins align in the same direction for increasing the polarization. In this case, it is possible to orientate the information in a precise direction. When the polarization gets to zero the system goes from ferroelectric to disorderly or paraelectric (PE) state because the spins are oriented in several directions where the information has not easily controlled.

Many works on ferroelectric proprieties of MTs have been done to better characterize the system. The piezoelectric properties of the microtubule were first discovered by Athenstadt et al. [24], He was looking for piezoelectric

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effects in living systems. The measurement of its piezoelectric properties and the subsequent classification as a piezoelectric polymer declared the existence of a permanent electric dipole on the microtubule. Brown et al. [25] re-examined the ferroelectric model of microtubules by showing the condition that the ferroelectric properties are important for the microtubule dynamic, and that microtubule can be affected by the transient endogenous electric fields of living cells. Pokorrny et al. [26] showed that the vibrations produced in the cell can generate an external electric field that influences certain proteins of the cell such as microtubules. In 2004, Chen Ying et al. [15] approached MTs as a one-dimensional ferroelectric system and describe the nonlinear dynamics of dimers of electric dipoles in a protofilament of the microtubule by virtue of the double-well potential, where they study MTs in the absence of the external electric field produced by other filaments in the cytoskeleton. They show that the ferroelectric to paraelectric FE-PE transition in the system occurs only through temperature. In 2005, Chen Ying et al. [27] studied the nonlinear dynamics of microtubules in the presence of a collective external electric field around the microtubules produced by vibrations inside the cell and showed that this electric field makes it possible to control the microtubule. In 2011, Cifra et al [28] measured the electric field generated by the modes of longitudinal vibration of axial microtubules in the dynamics.

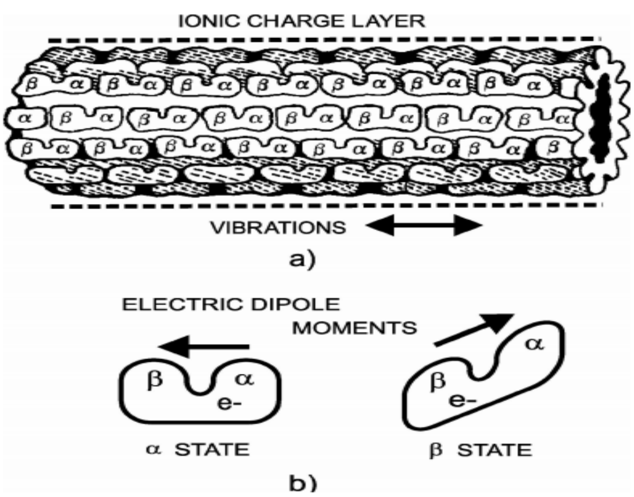


Figure 1. (a) Microtubule formed by protofilaments composed of tubulin heterodimers. (b) Heterodimer in α and β conformation state; the arrows denote the vectors of the electrical dipoles [14]

But none of these works properly explain how to control the information in the precise direction, more precisely how to increase or decrease polarization in MTs systems. Knowing that chemical displacement and anisotropic interaction can affect the direction of the signal propagation, we are looking at the effects of spin-spin coupling and anisotropic coupling on the dynamic of spins that form MTs. Moreover, the value and the direction of the electric field also affect the polarization, so in addition to previous points, we plan to characterize the polarization according to the transversally and longitudinally of the electric field. The paper is organized as follows: in section 2 we describe MT's system in terms of Hamiltonian, results, and discussions are presented in section 3 and section 4 concludes.

2. Model and Calculations

According with the work proposed by Chen Ying *et al.* [15] and that of Cifra et al. [28], we consider MT as a nonlinear ferroelectric chain made up of N pseudo-spin sites where anisotropic interaction [29,30] is taking into account. And then, we define the system using the Hamiltonian of the ferroelectric chain as:

$$H = -\Omega^x{}_i \sum_{i=1}^{N} S_i{}^x - \frac{1}{2} J \sum_{\prec i,j \succ}^{N} S_i{}^z S_j^z - \frac{1}{2} D \sum_{i=1}^{N} \left(S_i{}^z\right)^2 - 2\mu E \sum_{i=1}^{N} S_i{}^z \quad (1)$$

The first term represents transverse energy associated with the transverse field Ω^x. S_i And S_j represent the pseudo-spin respectively in site i and site j with $S_i = \pm \frac{1}{2}$. The second term characterizes the nearest -neighbor exchange interaction energy between the spin of the site i and the spin of the site j, with an interaction coupling $J > 0$. The notation $< i, j >$ meaning that the sum is restricted to the nearest-neighbor pair of pseudo-spin, each pair being counted only once [31]. The third term represents anisotropic interaction, where D is the anisotropic coefficient along the z-axis [32,33]. The last term represents the longitudinal external electric field and μ denotes the electric dipole moment.

Using the mean-field approximation (MFA) [15,34,35] we compute the effective Hamiltonian of the system using $S_i = (S_i{}^x, S_i{}^y, S_i{}^z)$ as a vector, its components are three Pauli matrices of the pseudo spin. Assuming that the density matrix ρ of the many-body system equal to the product of the single-particle density matrices ρ_i expressed as:

$$\rho_i = \left(Z_i\right)^{-1} \exp(\beta \sigma_i . S_i) \quad (2)$$

Where $\beta = \left(K_B T\right)^{-1}$ with k the Boltzmann constant, T the temperature and Z_i the partition function of a single-particle express as [15]:

$$Z_i = Tr \exp(\beta \sigma_i . S_i) = 2ch(\frac{1}{2} \beta \sigma_i) \quad (3)$$

Since σ_i denotes the effective field exerting on S_i defines as:

$$\sigma_i = -\frac{\partial \langle H \rangle}{\partial \langle S_i \rangle} \quad (4)$$

With $\langle H \rangle$ the thermodynamic expectation value of the Hamiltonian H.

By using the sum over nearest-neighbors defined as $\sum_{\prec i,j\succ} \to \frac{1}{2}\sum_{i=1}^{N}\sum_{j\in nn(i)}$, where the factor of $\frac{1}{2}$ is to avoid double counting pairs of sites and $nn(i)$ denotes nearest-neighbors of i. Since there is no explicit j dependence inside the summation, this inner sum is simply and $\sum_{j\in nn(i)} = q$ where the coordination number q is equal to the number of neighbors of any given site.

The value of q depends on the dimension of the system, for example, for a $1D$ lattice, $q = 2$; for a $2D$ triangular lattice, $q = 4$; for a $3D$ square lattice, $q = 6$. Assuming all these assumptions and consider $< S_j^{\,z} >=< S_i^{\,z} >$, the final expression of the effective field is given by:

$$\sigma_i = \left(\sigma_x, \sigma_y, \sigma_z\right) = \left(\Omega^x, 0, \left(D + J\frac{q}{4}\right)\sum_j < S_j^{\,z} > +2\mu E\right) \quad (5)$$

Eq.(5) can be recast as follow:

$$\begin{cases} \sigma_z = \left(D + J\frac{q}{4}\right)\sum_j < S_j^{\,z} > +2\mu E \\ \sigma_x = \Omega_x \\ |\sigma_i| = \sqrt{\Omega_x^{\,2} + \left(\left(D + J\frac{q}{4}\right)\sum_j < S_j^{\,z} > +2\mu E\right)^2} \end{cases} \quad (6)$$

By using Eq.(5), the effective Hamiltonian for the single-particle is:

$$H_{MFA} = -\frac{\partial\langle H\rangle}{\partial\langle P_i\rangle}.S_i = -\sigma_i.S_i \quad (7)$$

The thermodynamic expectation value of S_i is expressed as:

$$\langle S_i\rangle = \frac{TrS_i\exp(-\beta H_{MFA})}{Tr\exp(-\beta H_{MFA})} \quad (8)$$

Using Eq.(8), the coordinates of the pseudo-spin are as follow:

$$\begin{cases} \left\langle S_i^{\,x}\right\rangle = \frac{1}{2}\frac{\sigma_x}{|\sigma_i|}\tanh(\frac{1}{2}\beta|\sigma_i|) \\ \left\langle S_i^{\,y}\right\rangle = 0 \\ \left\langle S_i^{\,z}\right\rangle = \frac{1}{2}\frac{\sigma_z}{|\sigma_i|}\tanh(\frac{1}{2}\beta|\sigma_i|) \end{cases} \quad (9)$$

The total polarization P of the system is proportional to the thermal mean of the pseudo spin which is well defined in Ref. [33] by:

$$P^{\lambda} = 2N\mu < S_i^{\lambda} > \quad (10)$$

Since $\lambda = x, y, z$ and N represents the number of dimers in the microtubule and μ designates the single electric dipole.

Using Eq (10), the expressions of longitudinal polarization and susceptibility for the system are respectively giving by:

$$P^z = 2N\mu < S_i^z > \quad (11)$$

And

$$\chi = \frac{\partial P}{\partial E|_{E=0}} \quad (12)$$

3. Results and Discussions

In this section, we will compute numerically the longitudinal polarization and the electric susceptibility under the influence of various parameters such as spin-spin interaction, anisotropic interaction, and external field. Temperature greatly influences the dynamics of MTs and its variations show complex phenomena in living systems [36]. So, we will plot the polarization and the susceptibility as a function of temperature. Our main goal is to study the influence of these parameters on the transition of the ferroelectric phase to the paraelectric phase in the MT system.

In Fig.2, we have plotted the temperature dependence of the longitudinal polarization (Fig.2a) and the susceptibility (Fig.2b) in the absence of the external electric field at different values of the coupling constants of the tubulin dimers considering a specific value of the transverse field $\Omega = 1.5$.

It is shown that the polarization is a decreasing function of environmental temperature (Fig.2a), meaning that spins that form MT have the tendency to depolarize when the temperature of the system increases. High temperatures bring the system in PE state and mess up the orientation of the information in a specific direction. By considering the variations of coupling constantly related to spin-spin interaction and the anisotropic interaction, it is shown that the increase of coupling constant in the tubulin dimers leads to an increase in longitudinal polarization. Meaning that the increase of coupling constant tends to bring the system in a ferroelectric phase. The transition of the system from FE to PE will be delayed when the chemical displacement and the anisotropic interaction between the spins increase, the same results were obtained in [33].

In Fig.2b, the susceptibility dependence on temperature shows two behaviors, an increase behavior at low temperatures and a decrease behavior at high temperatures supposing that the MT system has a strong capacity to polarize at low temperatures; this result is in agreement with the result previously obtained in Fig.2a. For each value of the coupling constant, one can observe the critical point of susceptibility corresponding to the point where the polarization decreases to bring the system toward PE state. Moreover, these critical points correspond to critical temperatures that increase with increase the coupling constant. At high temperatures, the susceptibility is identical for the different values of the coupling constant, meaning that the coupling constant does not affect the polarization state of the system.

In Fig.3, we have studied the longitudinal polarization and the susceptibility in the absence of an external electric field at a specific value of the coupling constant $D+J$ by considering different values of the transverse field Ω. In Fig.3a, it is shown that by increasing the transverse field, the polarization decreases. So, the stronger is a transverse field and the weaker is the polarization of the MTs system. At high temperatures, the polarization is identical for the different values of the transverse field. Fig.3b shows the susceptibility as a function of temperature. It is observed that critical points disappear by increasing the transverse field. These results suggest that the presence of the transverse field in the system disturbs the orientation of the pseudo spins in the tubulin dimers and brings the system into PE state.

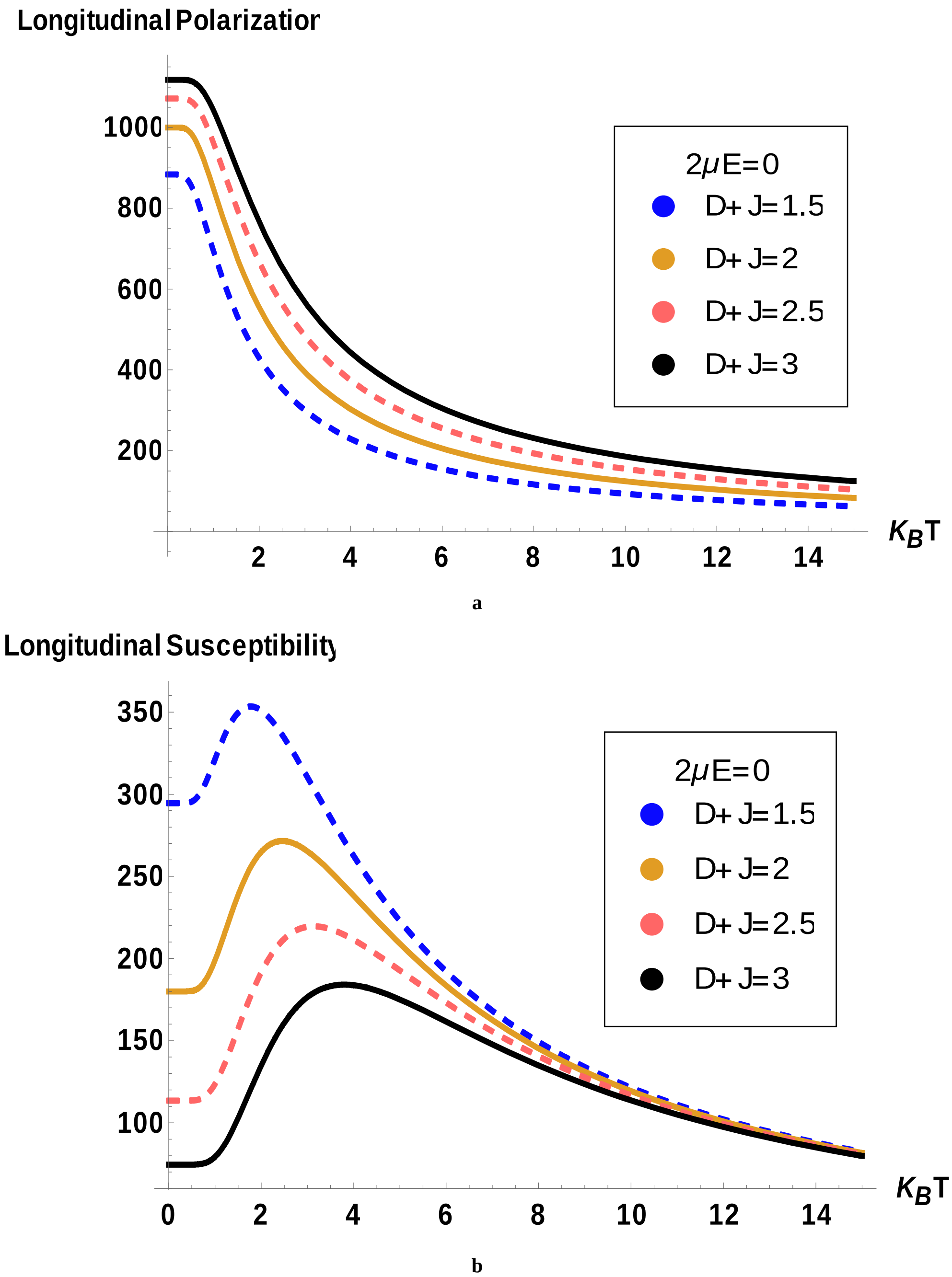
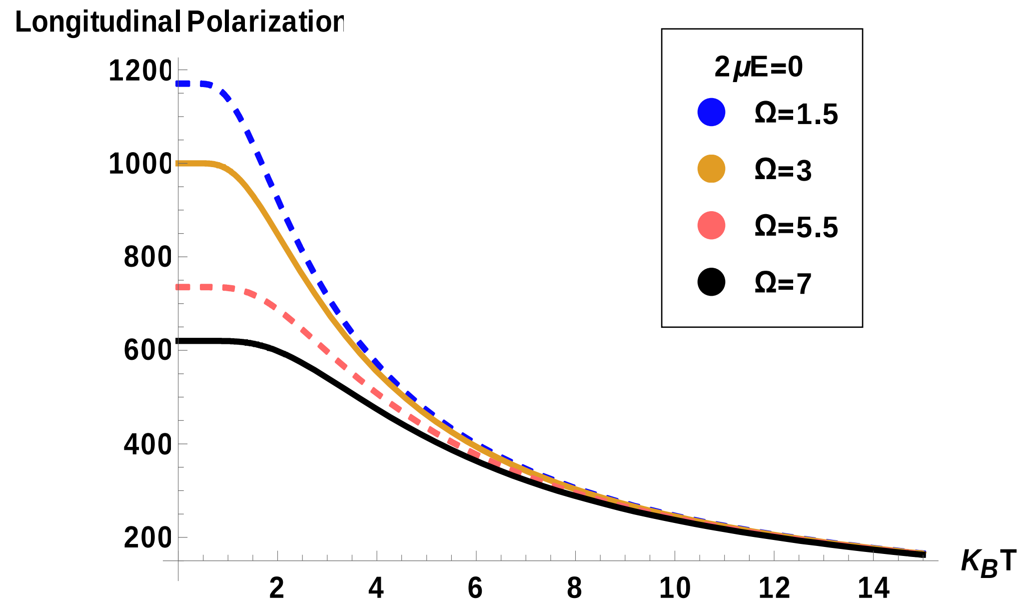


Figure 2. **a)** Longitudinal polarization as a function of temperature for different values of the coupling constants; **b)** Susceptibility versus temperature for different values of the coupling constants



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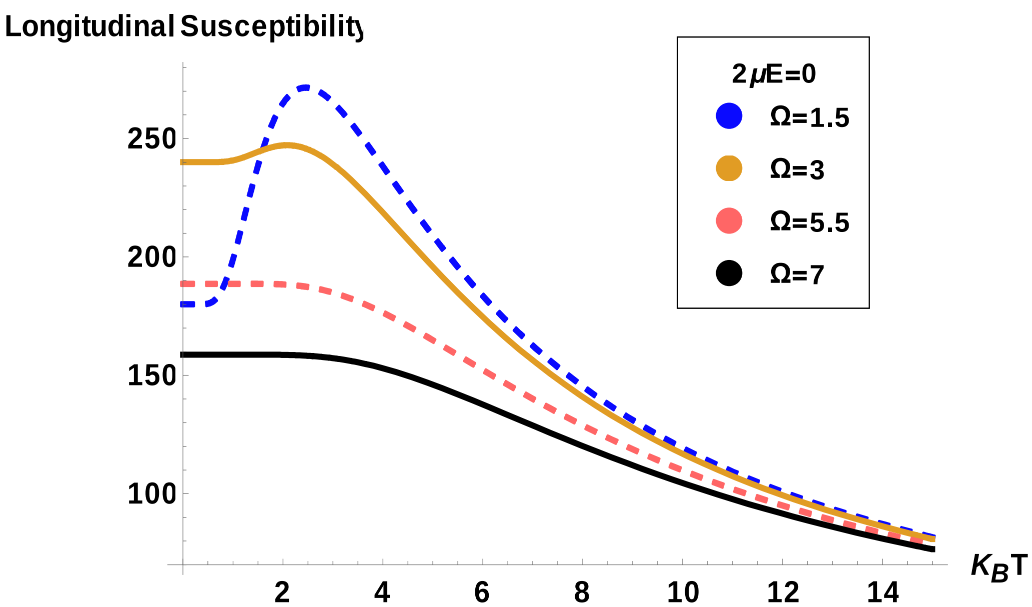

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Figure 3. **a)** Longitudinal polarization as a function of temperature for different values of the transverse field Ω . **b)** Susceptibility as a function of temperature for different values of the transverse field Ω

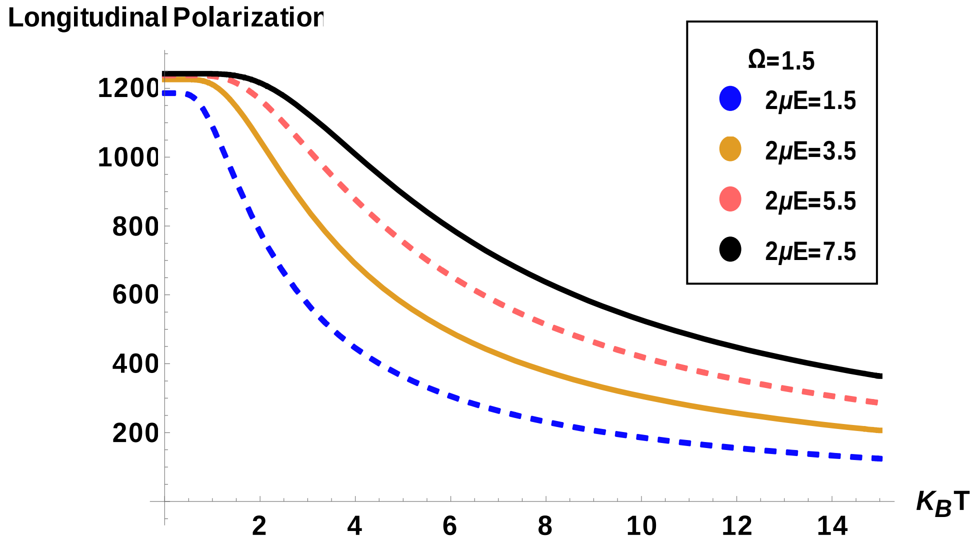
Fig.4 shows the behavior of the longitudinal polarization and the susceptibility in the presence of the external electric field $2\mu E$ for a transverse field Ω and the coupling constant $D+J$. The presence of a strong external electric field increases the polarization (see Fig.4a). This figure exhibits the same behavior that Fig.2a but, it is clearly shown that the range of polarization in this case, is higher than in Fig.2a. The behavior of the susceptibility is the same as that de Fig.2b. But in the presence of an external electric field, the critical temperatures are higher than those in Fig.2b. Meaning that the external electric field keeps the system in FE state [37]. In this case, the transition from FE to PE occurs later than in the absence of an external electric field.

Fig.5, presents the longitudinal polarization as a function of the external electric field at constant temperature $K_B T = 1.5$ and a given transverse field $\Omega = 1.5$. It is shown that the polarization increases by increasing the coupling constant. If the interaction between pseudo spins that form the MT changes when the external electric field varies, the system exhibits the hysteresis phenomenon. This result confirms the ferroelectric and nonlinear character of the MT system.

Fig.6, presents the variations of the longitudinal polarization under the influence of the external electric field for a given value of interaction coupling $J+D=1.5$, at constant temperature $K_B T = 1.5$ by varying the transverse field Ω. It is observed that the increase of the transverse field decreases the longitudinal polarization. So, increasing the transverse field destroys the hysteresis of the system.

4. Conclusions

In this work, by assuming microtubule system as an ensemble of N pseudo spins, we computed the longitudinal polarization and susceptibility using the mean-field approximation (MFA) in the absence and presence of the external electric field. In order to control the orientation of information in a specific direction, we studied the system in the absence of an external electric field by considering the influence of spin-spin interaction, anisotropic interaction and constant transverse field. The results obtained show that the increase of coupling constant brings the system in a ferroelectric phase while high temperatures bring the transition to the paraelectric phase. This last result was also obtained by studying the influence of the transverse field at a constant interaction coupling. In the presence of an external electric field, the critical temperature increase more than in the absence of an external electric field. In this case, the system is maintained in the ferroelectric configuration and exhibited the hysteresis phenomenon that is destroyed by increasing the transverse field in the system. The external electric field can be used to control the direction of information in the microtubules. Thus, the transverse field and temperature promote the paraelectric phase while spin-spin interaction, anisotropic interaction and external electric field maintain the MT system in the ferroelectric phase.



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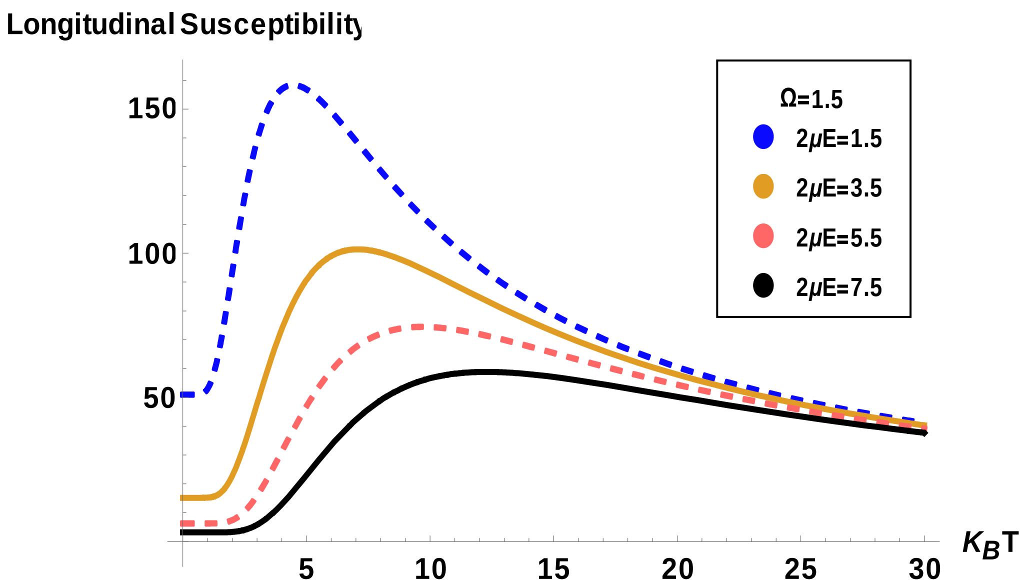

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Figure 4. a) Longitudinal polarization as a function of temperature for different values of the electric field $2\mu E$. **b)** Longitudinal susceptibility as a function of temperature for different values of the electric field $2\mu E$

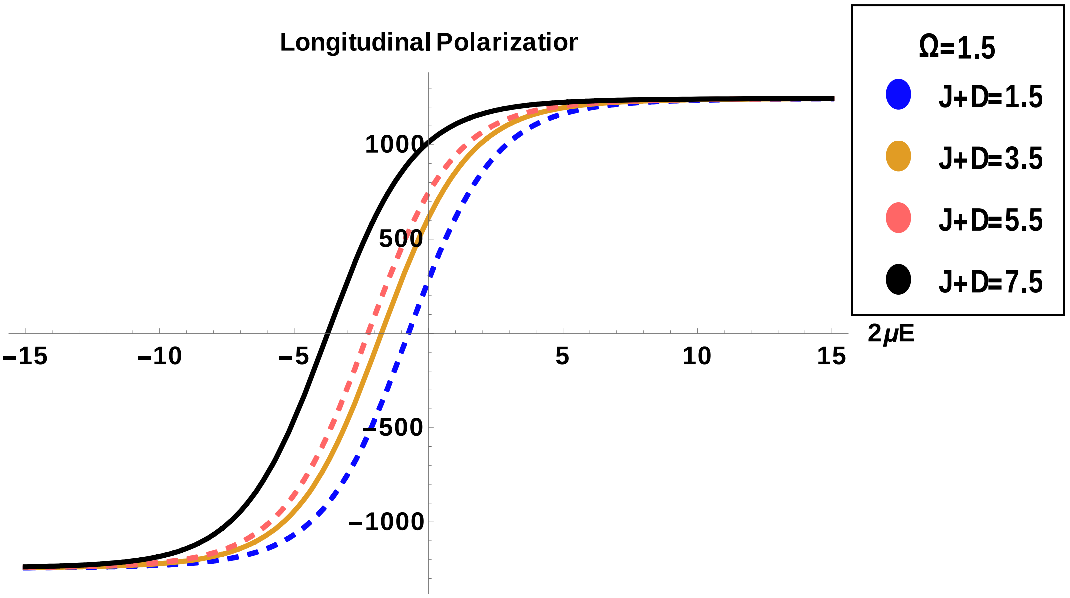

Figure 5. Longitudinal polarization as a function of the electric field $2\mu E$ at different values of coupling constant

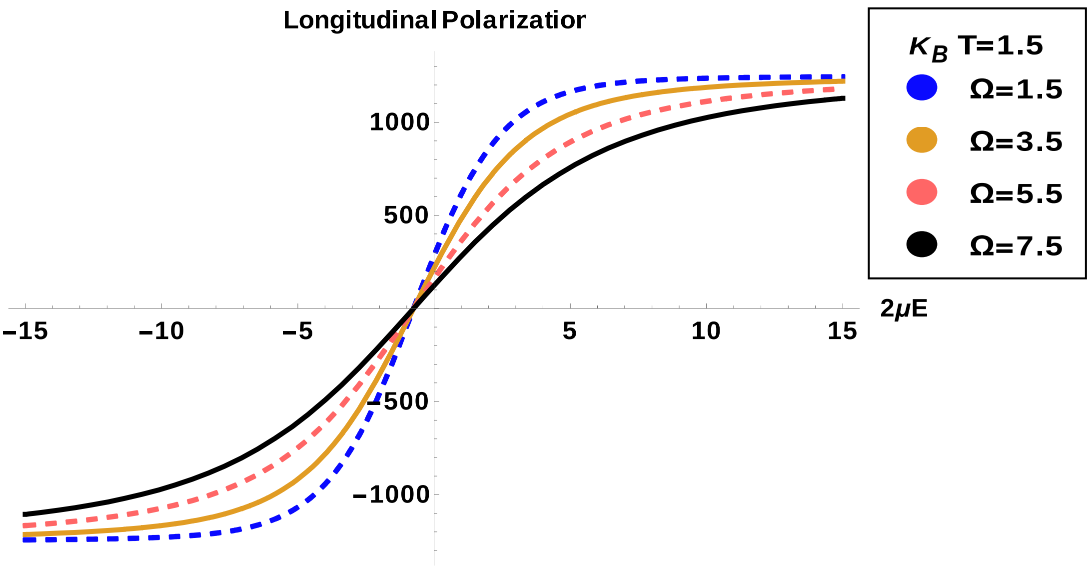

Figure 6. Longitudinal polarization as a function of the electric field $2\mu E$ at different values of the transverse field

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