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APPLICATION OF THE LAGRANGE EQUATION TO THE OSCILLATION OF THE PEPTIDE PLANE IN AMINO-ACIDS CHAIN

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Abstract. *We have made an attempt to simulate the oscillation of peptide planes – a planar formation in amino-acid chains in tubulin subunits. Because of Curie simmetries in living organisms we can use capability of classic Lagrange equations application. The newly developed method gives possibility for calculation tree perpendicular proper frequencies for each atom in peptide plane. The influences of four contacting and six neibouring atoms can be settle up accounts. The effect of whole in chain oscillations appears explicitly, with the consequence that there does not exists two identical oscillating pictures in chain of 450 amino-acids in tubulin subunits.*

Key words: *Lagrange equation, oscillation, biophysics, amino-acids chain, peptide plane.*

1. INTRODUCTION

The amino-acids are losing one molecule of water in the process of connecting into amino-acid chain, so they can be presented as quasi 1-D object in figure 1. However, the peptide bond is planar, then the polypeptide chain has only two degrees of freedom per residue. The skeleton atoms of nitrogen and carbon N-C_α-C_β are laterally connected with atoms of oxygen and hydrogen, and amino-acid tails (R).

Microtubules in living organisms are specially interested from the point of view of the information physics theory. The information physics encounters a synergetic theory of classical mechanics, quantum mechanics and theory of information. Using this new scientific paradigm it is found that microtubules with clathrins and water clusters in living cells are major biomolecular devices which satisfy synergy principles of information physics [1], [2].

The mass numbers for amino acids and their numeric representations in alpha and beta tubuline subunits are presented in Table 1. A basic skeleton of each amino-acid has

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the same mass number (56 D), but the mass of amino acids tail is from 1 to 130 D, where $1D = 1{,}67 \cdot 10^{-27}$ (kg). The second important difference between tails appears in form (Figure 2). Three main types of secondary structure of amino-acid are: helix, beta planes and random chains [6] [7], [8], [9]. Each one of them has its specific function in proteins. α tubuline monomer consists of 454 amino-acids while β tubulin consists 450, with total mass 50500 D and 50 230 D, respectively.

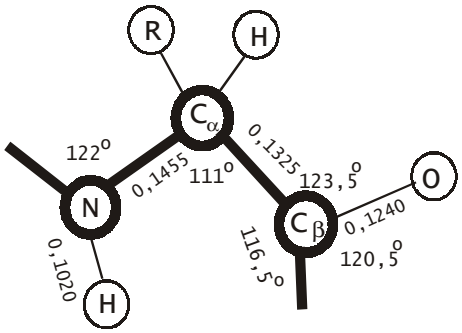

Fig. 1. Model of amino-acid in chain. Distances between atoms are given in nanometers, while the angles are in degrees. Skeleton of atoms which make protein chain is given as a bold line.

Table 1. Mass numbers of amino-acids (m), their tails (m_R) and their number in alpha and beta tubuline subunits

A.A.	M	R	E	C	I	S	H	V	G	Q
m	131	157	128	103	113	87	137	99	57	128
m_R	75	101	72	47	57	31	81	43	1	72
α	10	21	39	12	26	23	13	34	37	16
β	18	22	36	8	18	28	9	34	39	22
A.A	A	N	W	L	Y	P	D	K	T	F
m	71	114	186	113	163	98	114	129	101	147
m_R	15	58	130	57	107	42	58	73	45	91
α	38	16	4	31	19	20	28	19	29	29
β	29	23	4	32	16	21	28	15	30	23

2. MODEL OF PEPTIDE PLANE OSCILATION

Proteins are systems with relatively small number of atoms, comparing to thermodynamic systems. In spite they have discrete structure, we can apply Curie limit symmetry [1] which gives a continuous system. In other words, we can use both - classic and quantum physics approach.

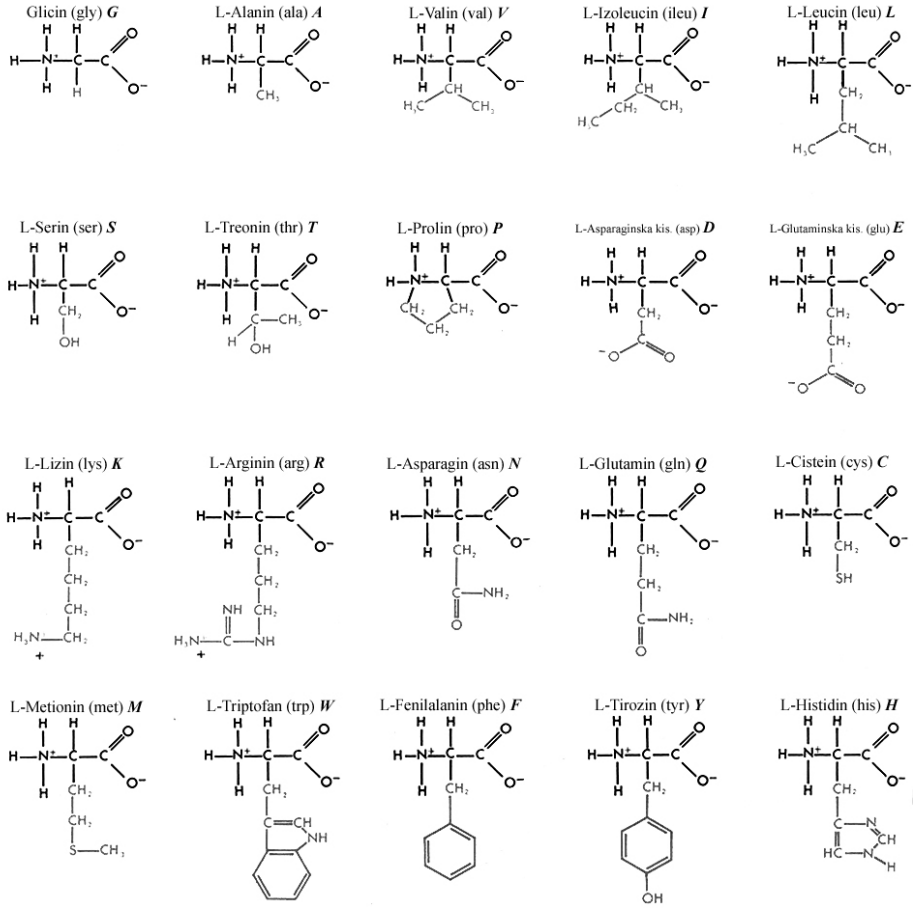

Fig. 2. Table of amino-acids with their notation and structural formulas [12]

We apply classic Lagrange model [3],[4] because we are not interested in the oscillations of electrons, but the oscillation of atoms, as parts of system. We have considered that space is filled, so each atom has, beside basic connections, several lateral connections too. They can be much weaker than basic connections, in the chain. Also, we have to bear in mind that dominant connections in biological systems [5] are different types of electromagnetic interactions. We applied Lagrange equations for moving, on the limited chain of amino-acids.

Peculiarities of bio-systems are:

(1) greather distance between atoms, than in free molecules,

(2) Coulombic interaction, and

(3) Hydrogen bonding.

what we have included in a model, for each atom. To compare with classical approach, the two more imporant changes in procedure are:

(1) transition from atom position as variable, to the deviation of equilibrium position as variable,

(2) consider that chain is limited and in contact with enviroment.

Our solution is equivalent to the solution of Klein-Gordon equation for continuum, because of very small distances between atoms (more than about ten picometres) and very big number of atom in chain (more than million).

For each atom, real connections can be presented in a model, as shows in figure 3. We can see that four equivalent atom connections are in mutually normal direction, in action to every atom. New six atoms with its connections are indirectly included in deterination of proper frequency. So we have in model four connecting and six neibouring atoms,which gives the summary of ten. This gives that our model can be very close to the realistic one.

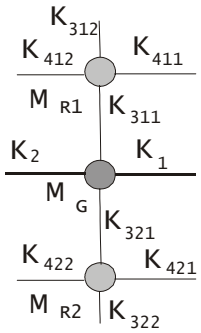

Fig. 3. A model of oscillator with all necessary values for calculation: K - coefficient of connection, M_G, M_R - mass of "head" and of "tail", K_1,K_2 - connections along basic oscillating channel.

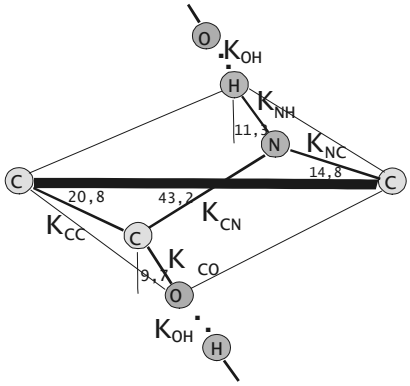

Fig. 4. Peptide plane with diagonal of oscillating along skeleton and angles between connections.

If atom in connection is not in proposed directions in model that atom will be divided in two atoms with the same mass and new coefficients determined by actual, but modified with coefficients of angle.

The physical nature of Coulomb force, and balance of forces in opposite direction determines manner of combining coefficients as follows in eqn. (1) and (2). Coefficients K_{41}, K_{42} give possibility for calculation of longitudinal frequencies for latteral atoms, in similar way. Frequencies of oscillation for atom M_G in chain with N atoms, with two perpendicular modes, are determined by eqn. (3) .

$$\frac{1}{K_3}=\frac{1}{K_{31}}+\frac{1}{K_{32}},\quad \frac{1}{K_{31}}=\frac{1}{K_{311}}+\frac{1}{K_{312}},\quad \frac{1}{K_{32}}=\frac{1}{K_{321}}+\frac{1}{K_{322}}. \tag{1}$$

$$\frac{1}{K}=\frac{1}{K_1}+\frac{1}{K_2},\quad \frac{1}{K_{41}}=\frac{1}{K_{411}}+\frac{1}{K_{412}},\quad \frac{1}{K_{42}}=\frac{1}{K_{421}}+\frac{1}{K_{422}}\ . \tag{2}$$

$$\omega_G^2=\frac{K_3}{m_G}+\frac{K}{m_G}4\sin^2\frac{n\pi}{2(N+1)}=\omega_{GY}^2+\omega_{GX}^2. \tag{3}$$

In figures 4 and 5, the peptide plane is presented with the real positions of atom and as planar quasi-structure with lengths (in nanometers) and angles (in degrees).

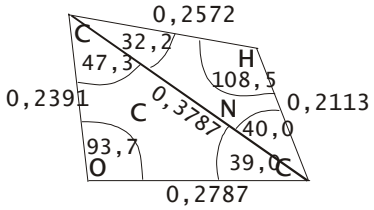

Fig. 5. Lengths and angles of peptide plane. For hydrogen atom position is determined from balance of forces that affect it.

3. DISCUSSION

The peptide plane consists of a forward part of one and a backward part of another amino-acid. It is a plane structure which acts as a quasi-particle**,** because deformed clouds of electrons give an additional strength. Beside that, the harmonization of electric force and gravity [10], [11] in living matter makes distances between atoms larger than in non living matter [5].

The tail is connected normal to direction except for proline, and tails oscillate along the third degree of freedom.

We calculated the oscillation of peptide plane atoms, along a large diagonal (*x*-axis), along its normal (y-axis) and along a tail normal to the peptide plane (*z*-axis). The oscillation of atoms on vertices position O-C-H-C in three planes: *xy*, *yz*, *zx* is graphically presented, as well as the amplitude change in time.

For each amino-acid in chain, choosing of code number takes into account an organizational structure (helix, plane, random array). Because of the whole effect to oscillating frequency, two amino-acids with the same oscillating picture can't exist (see figures 6 and 7).

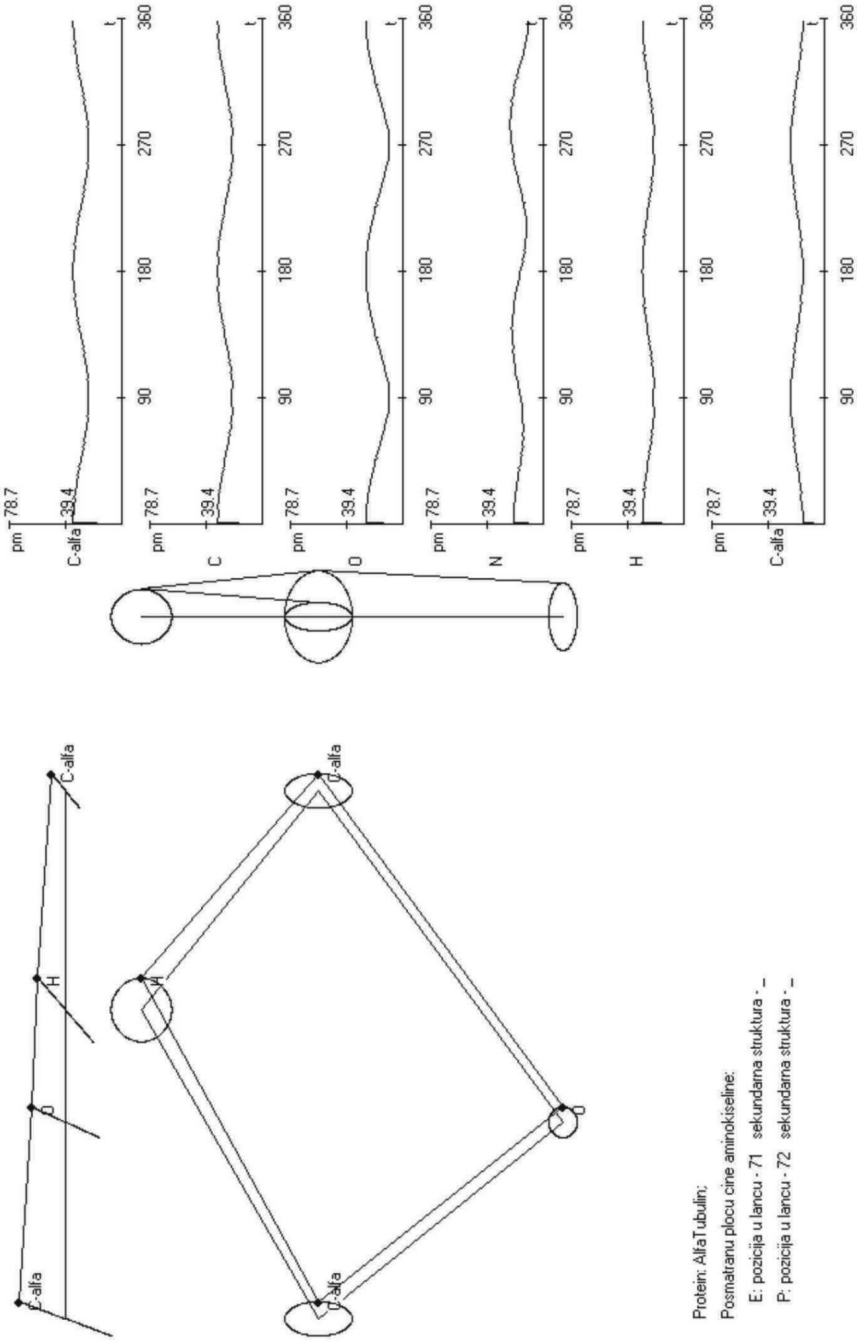

Fig. 6.a. Oscillations of peptide plane determined by parts of E and P, at positions 71-71 in alpha tubuline, in helix.

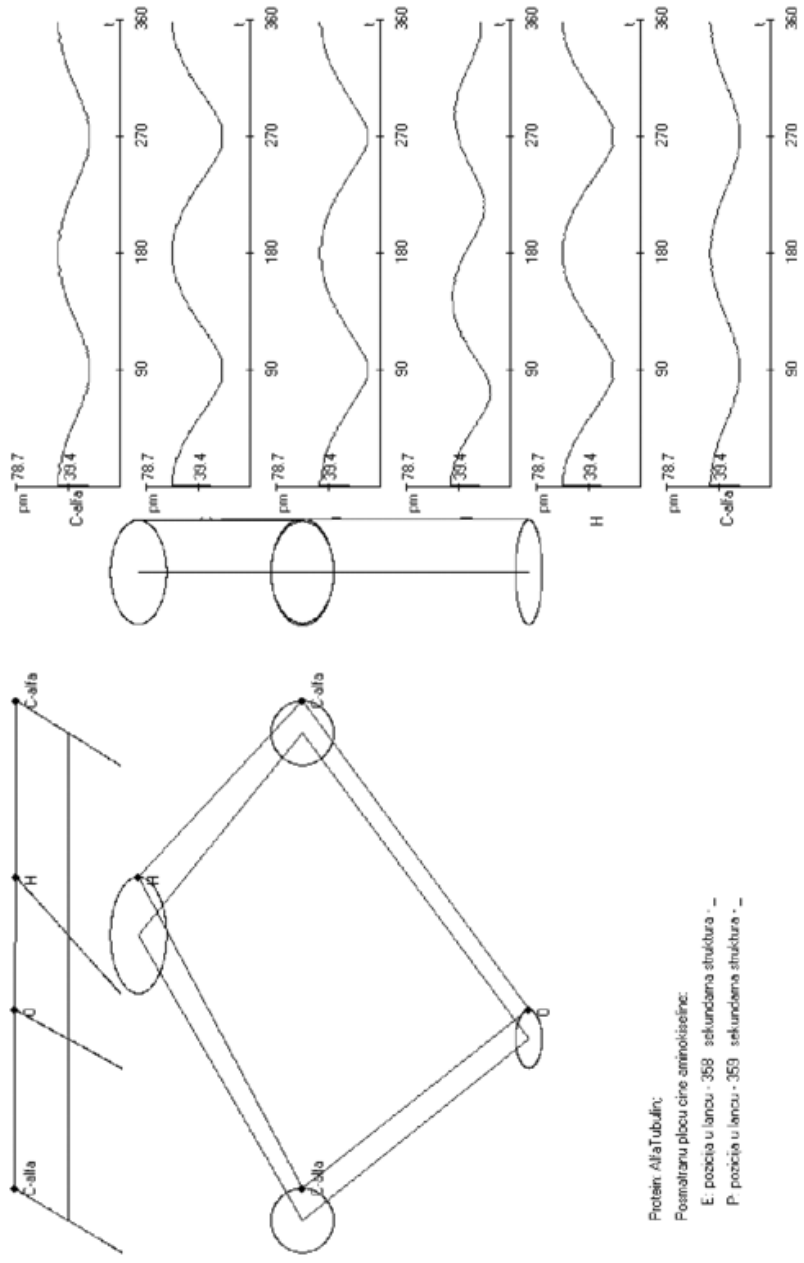

Fig. 6.b. Oscillations of peptide plane determined by parts of amino-acid E and P, at positions 358 -359 in alfa tubuline, in random structure.

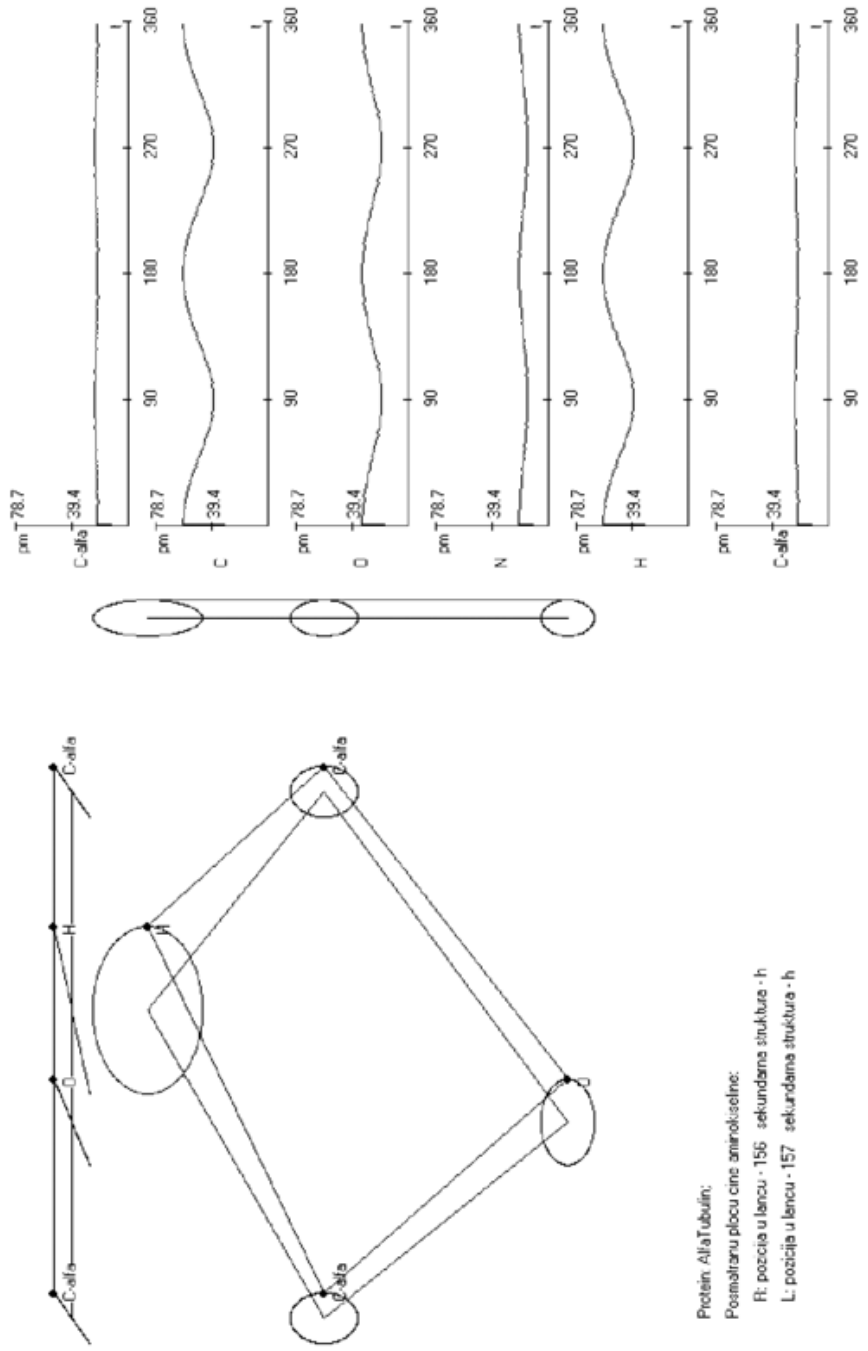

Fig. 7.a. Oscillations of peptide plane determined by parts of amino-acid R and L, at positions 156-157 in alfa tubuline, in helix.

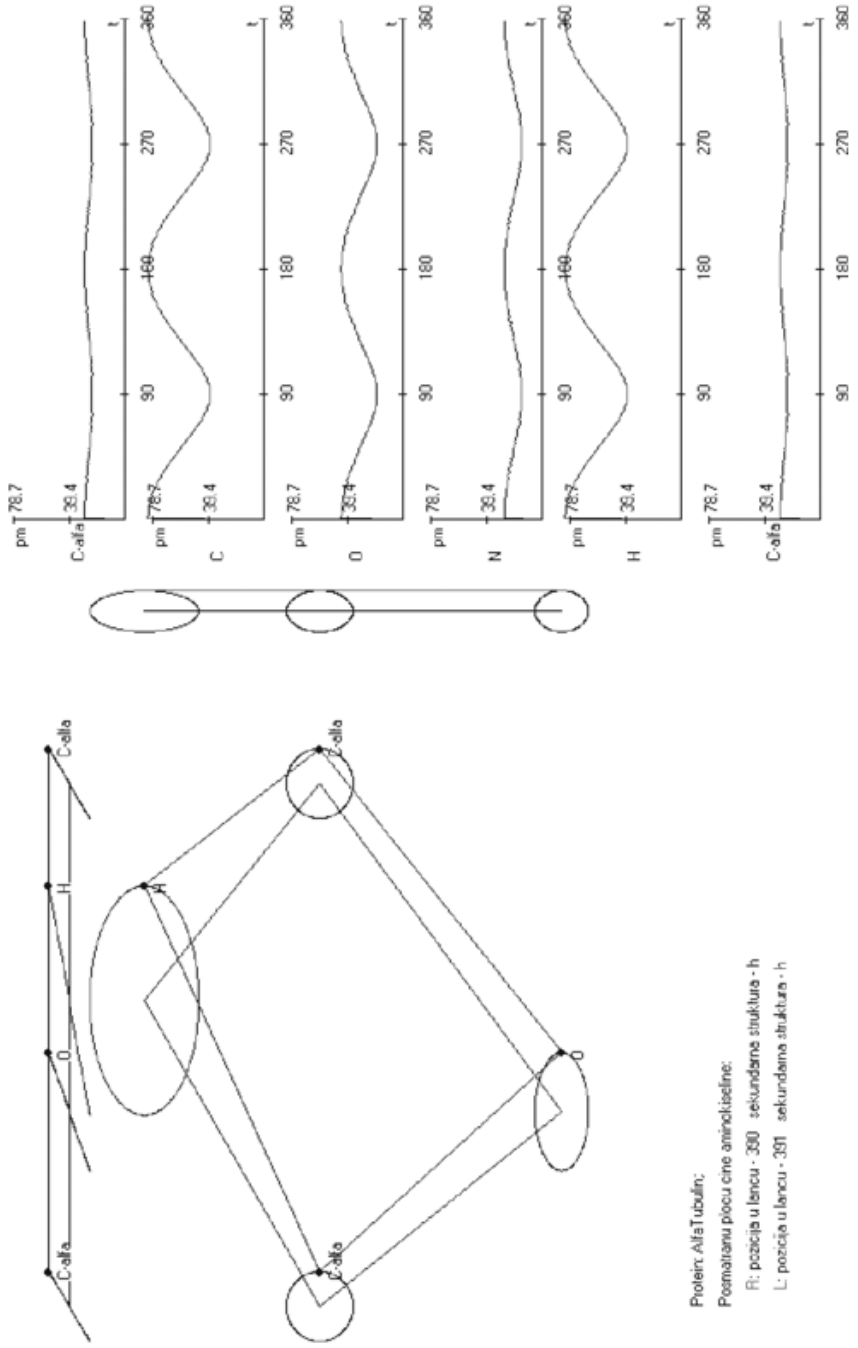

Fig. 7.b. Oscillations of peptide plane determined by parts of amino-acid R and L, at positions 390-391 in alfa tubuline, in helix.

4. CONCLUSION

The model presented here gives possibility to discover oscillating pictures of chain with a few thousand atoms. We can calculate frequencies for each atom in skeleton or associate them to skeleton, but here we follow the peptide-plane oscillation.

The richnes of data can be further used in different purposes. We assume first to extract the statistics of energy and entropy for peptide plane as quasi-particle.

In the next step we shall focus our attention on these caracteristics of system, because of border symmetries there exsists the opportunity with a real chance that unexpected properties can be found for peptide plane as quasi-particle.

Generally, this model is applicable in many other biological structures, and presents a new approach to analyze behaviour of biomolecules by influence of electromagnetic and mechanical stress.

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PRIMENA LAGRANGE-OVIH JEDNAČINA NA OSCILOVANJE PEPTIDNIH RAVNI U AMINO-KISELINSKOM LANCU

Aleksandar Tomić, Željko Ratkaj, Djuro Koruga

Učinjen je pokušaj simuliranja oscilovanja peptidnih ravni – ravanskih formacija u aminokiselinskom lancu u subjedinicama tubulina. Zbog važenja Curie-simetrija u živim organizmima bilo je moguće iskoristiti pogodnost primene klasičnih Lagrange-ovih jednačina. Novi uvedeni metod daje mogućnost za izračunavanje tri medjusobno normalne sopstvene frekvencije za svaki atom u peptidnoj ravni. Uticaji četiri kontaktna i šest susednih atoma mogu se obračunati. U oscilovanju lanca pojavljuje se eksplicitno "efekat celine", sa posledicom da ne postoje dve identične slike oscilovanja u lancu od 450 aminokiselina u subjedinicama tubulina.