**Research article**

# Three-level discrete quantum model of ideal water chain in a constant magnetic field

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## Abstract

In work is presented quantum – mechanical model of movement of the five–molecular repeating part of a ideal one–dimensional periodic water chain in a constant magnetic field concerning it. Angular values between hydrogen communications in molecules of water rely not such as in amorphous structure and not such as in crystals of an ice. Realizations of such structure of water is hypothetically possible only in special conditions. Intermolecular interaction and change of hydrogen communications are modeled as restrictive conditions (as communications in mechanical system) according to Bernal – Fowler rules at constancy of interaction potential and with a condition of invariance of mass-center position of repeating part in chained structure of water. The model is realized by the obvious computing scheme and as a result quantum levels and the probabilities of quantum transitions for such water structure are found.  **Copyright © acascipub.com, all rights reserved.**

**Keywords:** chained structure of water, magnetic field, quantum levels, quantum transitions

## Introduction

Let's consider one–dimensional periodic chained structure of water consisting from five–molecular repeating parts formed by the Bernal - Fowler rules [1] (see on figs. 1 – 11 – « $^O$ » – designates atom of oxygen; solid line is intermolecular communications with atoms of hydrogen; more details explaining it, will be given below). Angular values between hydrogen communications in four molecules of water are assuming to equal $\pi/3$

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and the physical aspects of realization of it we shall discuss in conclusion of the work. The moment of forces $M$ acting on the repeating part (in further it will named as «water sublimer») in a homogeneous and constant magnetic field is follows ( $r_k$ is the radius-vectors describes line of moving of atom of hydrogen, definition of its initial and final points will be given below).

$$M = \sum_k [r_k, F_k] = \frac{e}{c} \sum_k [r_k, [B, V_k]] = \frac{e}{c} \left( B \sum_k (r_k, V_k) - \sum_k V_k (r_k, B) \right)$$

Here summation is conducted on an index « $k$ » numbers of moving atoms of hydrogen of all molecules of sublimer; the bracket $[,]$ designate vector multiplication; $(,)$ scalar multiplication; $e, c$ - an elementary charge and speed of light; $B$ – a vector of a magnetic induction; $F_k = \frac{e}{c} [B, V_k]$ – the Lorenz forces acting to core of hydrogen atom moving with a speed $V_k$. The cloud of an external electronic layer of a molecule is considered thus conditionally motionless. Angular speeds $\omega_k$ of this movement are entered, thus $V_k = [\omega_k, r_k]$.

Then expression for the moment of forces is $M = -\frac{e}{c} \sum_k [\omega_k, r_k](r_k, B)$.

Further we shall consider the values having sense of near to moments of impulses (almost kinetic moments) which get atoms of hydrogen $p_k = m_H R^2 \omega_k$ , here $m_H$ - mass of atom of hydrogen; $R$ – the characteristic size of water sublimer (average distance between atoms of oxygen); then:

$$M = \frac{e}{m_H c R^2} \sum_k (r_k, B)[r_k, p_k] \tag{1}$$

**Materials and Method**

Now operation similar to averaging with weight multipliers is appear but it will be made by vector multiplication (instead of usual scalar) i.e. are entered values:

$$H = \frac{e}{m_H c R^2} \sum_k (r_k, B) r_k \ ; \ p = \frac{[M, H]}{H^2} \tag{2}$$

If to designate $H_k = \dfrac{e}{m_H c R^2}(r_k, B) r_k$ then (2) is rewriting as $p = \dfrac{\left[ \sum\limits_k [H_k, p_k], \sum\limits_k H_k \right]}{\left( \sum\limits_k H_k \right)^2}$ , and this

expression has analogy of a weight average.

Expression (1) $M = \sum\limits_k [H_k, p_k]$, under condition of $(M, H) = 0$ and in view of (2) gets a kind

$M = [H, p]$. Really: $M = \left[ H, \dfrac{[M, H]}{H^2} \right] = M - H \dfrac{(M, H)}{H^2}$

It is necessary to explain condition $(M, H) = 0$, its consistence and the cases of its executing. We concretize it (expression $( , , )$ means the mixed multiplication of vectors).

$(M, H) = \dfrac{e^2}{m_H c^2 R^2} \sum\limits_{k,l} (r_k, B)(r_l, B)(r_k, \omega_k, r_l) = \dfrac{e^2}{m_H c^2 R^2} \sum\limits_{k,l} (r_l, B)(r_k, B)(r_l, \omega_l, r_k)$   that   is

$(M, H) = \dfrac{e^2}{m_H c^2 R^2} \sum\limits_{k<l} (r_k, B)(r_l, B)(r_k, \omega_k - \omega_l, r_l)$. Further under conditions $(V_k, r_k) = 0$ angular

speeds $\omega_k = \dfrac{[r_k, V_k]}{r_k^2}$ then $V_k = \dfrac{[[r_k, V_k], r_k]}{r_k^2} = \dfrac{[r_k, [V_k, r_k]]}{r_k^2} = V_k - \dfrac{(V_k, r_k) r_k}{r_k^2}$ and:

$(M, H) = \dfrac{e^2}{m_H c^2 R^2} \sum\limits_{k<l} (r_k, B)(r_l, B)\left( r_k, \dfrac{[r_k, V_k]}{r_k^2} - \dfrac{[r_l, V_l]}{r_l^2}, r_l \right)$

Linear speeds let to define as $V_k = \dfrac{\rho_k}{\tau}$ here $\rho_k$ - vectors of displacement of atoms of hydrogen at

movement of sublimer (on figs. 1 – 11 which will be explained below, these vectors are shown by arrows),
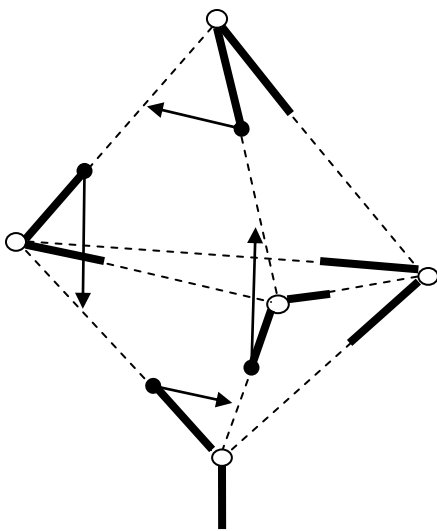
$\tau = \dfrac{m_H c}{e|B|}$ a characteristic time scale, $|B|$ – the module of a magnetic induction. Thus:

$(M, H) = \dfrac{e^2}{\tau m_H c^2 R^2} \sum\limits_{k<l} (r_k, B)(r_l, B)\left( \dfrac{1}{r_k^2} ([\rho_k, r_k], [r_k, r_l]) + \dfrac{1}{r_l^2} ([\rho_l, r_l], [r_l, r_k]) \right) =$

$$= \frac{e^2}{\tau m_H c^2 R^2} \sum_{k<l} (r_k, B)(r_l, B) \left( \frac{1}{r_k^2} \begin{vmatrix} (\rho_k, r_k) & r_k^2 \\ (\rho_k, r_l) & (r_k, r_l) \end{vmatrix} + \frac{1}{r_l^2} \begin{vmatrix} (\rho_l, r_l) & r_l^2 \\ (\rho_l, r_k) & (r_l, r_k) \end{vmatrix} \right)$$
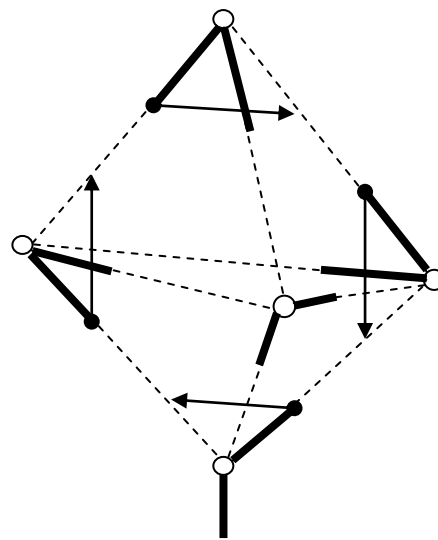
Further using the conditions $(\rho_k, r_k) = 0$ we continue equality:

$$(M, H) = -\frac{e^2}{\tau m_H c^2 R^2} \sum_{k<l} (r_k, B)(r_l, B)((\rho_k, r_l) + (\rho_l, r_k)) = -\frac{e^2}{\tau m_H c^2 R^2} \sum_k (r_k, B) r_k \sum_k (r_k, B) \rho_k$$



**Figure 1.** State 1 and transition number

$m = 1$ to state 4 ( $s = 2$ – type of transition)

**Figure 2.** State 2 and transition

$m = 2$ to state 1 ( $s = 2$ )

For satisfaction of the equation enough $\sum_k (r_k, B) r_k = 0$ and in view of that the «pole» $r_0$ from which

vectors $r_k$ are issued, is not determined, therefore it is possible to write down

$$\sum_k (r_k - r_0, B)(r_k - r_0) = 0 \tag{3}$$

as condition for searching $r_0$ from it.

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If to consider $r_* = \dfrac{1}{N}\sum_k r_k$ and $h_* = \dfrac{1}{N}\sum_k (r_k, B)r_k$ here $k = 1,..., N$ – number of moving atoms of

hydrogen (with communication depending on a state of sublimer) the equation (3) can be copied so:

$(r_0 - r_*)(B, r_0 - r_*) = r_*(B, r_*) - h_*$ Really

$$r_0 = \frac{\sum_k (r_k - r_0, B)r_k}{\sum_k (r_k - r_0, B)} = \frac{N h_* - N(B, r_0)r_*}{N(B, r_*) - N(B, r_0)} = \frac{((B, r_0) - (B, r_*))r_* + (B, r_*)r_* - h_*}{(B, r_0) - (B, r_*)} = r_* + \frac{(B, r_*)r_* - h_*}{(B, r_0 - r_*)},$$

from it follows, that the equation (3) has two complex conjugating solutions $r_0 = r_0^+, r_0^-$ «imaginary poles». That

fact demands the explanatory that real solutions $r_0^+, r_0^-$ do not exist.

For it we shall consider the coordinate axis which is passing through a point $r_*$, with a directing vector

$r_*(B, r_*) - h_*$, we shall designate $s_* = \|r_*(B, r_*) - h_*\|$. We shall admit of the laying of point $r_0$ on this axis, and

shall designate a projection $r_0 - r_*$ as $s_0$ i.e. $r_0 - r_* = (r_*(B, r_*) - h_*)\dfrac{s_0}{s_*}$. Then equation

$(r_0 - r_*)(B, r_0 - r_*) = r_*(B, r_*) - h_*$ in a projection to an axis will give $s_0^2 \sigma_* = s_*^2$ here

$\sigma_* = (B, r_*(B, r_*) - h_*)$.

The condition of existence of a real solution $r_0$ (i.e. real $s_0$) then is in the form of

$\sigma_* = \dfrac{1}{N^2}\left(\left(\sum_k (B, r_k)\right)^2 - N\sum_k (B, r_k)^2\right) > 0$. But this inequality contradict with $\left(\sum_{k=1}^{N} x_k\right)^2 - N\sum_{k=1}^{N} x_k^2 \le 0$

the true for any real numbers (for reach of equality $x_1 = ... = x_N$). Therefore if $\sigma_* < 0$ then in space of complex

vectors $r_k$ the numbers $s_0 = \pm i\dfrac{s_*}{\sqrt{-\sigma_*}}$ can be only imaginary (coordinates of vectors $r_0^-$ are complex

conjugating with $r_0^+$).

Now it is necessary to explain figs. 1 – 11. The structure of water sublimer is explaining by Bernal – Fowler rules (on the communication line between two atoms of oxygen there can be only one atom of hydrogen, and each atom of oxygen is connected with four atoms of hydrogen). These conditions define the kind of a sublimer ambiguously. Possible change of position of the "free" hydrogen communication line (the atom of oxygen in height joins with free hydrogen communication or they can exchange places). One example of such change of position with the advent of free hydrogen in opposite top is shown on fig. 11.

Two additional conditions are imposed for determination of sublimer motions: a constancy of potential of intermolecular interaction and an invariance of the mass-center position of sublimer in chained structure of water. First condition in assumptions of the given mathematical model (the skeleton of sublimer of water consists of two tetrahedrons and remains constant) is reduced to the sum of corners between intermolecular communications on all molecules of sublimer should be identical for all states of sublimer. The second – the sum of vectors of moving of atoms of hydrogen $\rho_k$ should be zero. These conditions limit an opportunity of change of positions of atoms of hydrogen in sublimer of water. At an invariance of positions of lines of molecular communications 30 variants of the interconnected displacement (without change of orientations of "free" hydrogen atom – it is already change in all chained structure of water) are possible. Direct and return transitions distinguish signs of vectors $\rho_k$ and initial positions of hydrogen communications therefore their transition numbers «$m$» has a different signs (with identifying of direct and inverse transitions we have 15 variants).

Thus six various states of sublimer are numbered conditionally (corresponds to numbers of figures $1 - 6$) i.e. the set of states of sublimer of water is a five-dimensional tetrahedron (has 6 tops and $C_6^2 = 15$ edges). Possible transitions between any two states are represented as moving along the edges of this tetrahedron. Thus transitions of three types are possible: the first – three atoms of hydrogen are displacing (example see on fig. 4); the second – four (figs. $1 - 3$); the third – seven (figs. $5 - 10$). These types are numbered by an index «$s = 1, 2, 3$» accordingly. On figures ten transitions are shown only, but the others can be received by analogy - the corresponding algorithm will be specified.
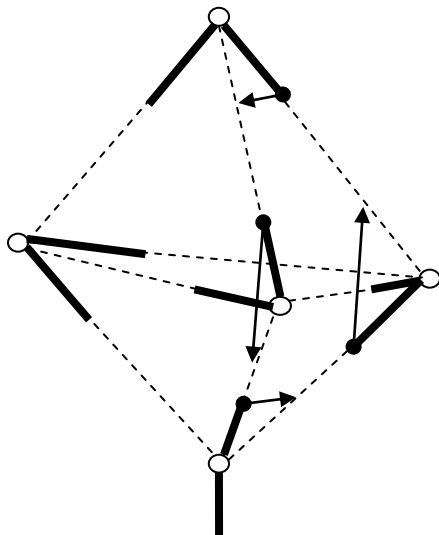


**Figure 3.** State 3 and transition

$m = 3$ to state 6 ( $s = 2$ )
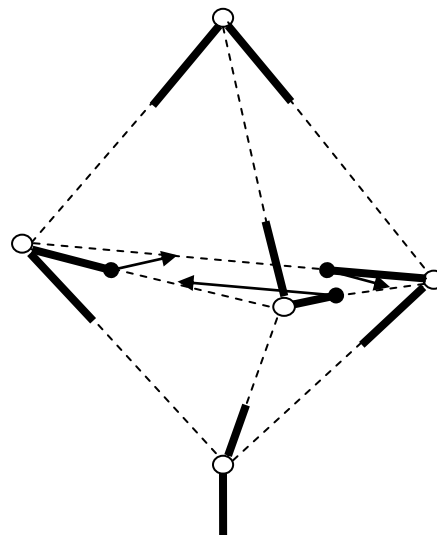
**Figure 4.** State 4 and transition

$m = 4$ to state 3 ( $s = 1$ )

So, if complex vectors $r_k$ are begin from any imaginary pole $r_0^+$ or $r_0^-$ how it has been using a condition $(M, H) = 0$ then consequence will provide $M = [H, p]$.

By analogy to a vector $M$ we shall consider a vector $\Omega = \sum_k \omega_k r_k^2 (r_k, B) = \sum_k (r_k, B)[V_k, r_k]$ as

already it was marked above $\omega_k = \dfrac{[r_k, V_k]}{r_k^2}$ under condition of $(V_k, r_k) = 0$. Now if to consider $V_k = \dfrac{\rho_k}{\tau}$ then

possible to write:

$$\Omega = \frac{e|B|}{m_H c} \sum_k (r_k, B)[r_k, \rho_k] = \frac{e}{m_H c R^2} \sum_k (r_k, B)[r_k, q_k] \; ; \; q = \frac{[\Omega, H]}{H^2} \tag{4}$$

Here $q_k = R^2 |B| \rho_k$ and it enables to write down expression $\Omega = \sum_k [H_k, q_k]$ similar (1) and then using

«vector weight averaging» is similar (2) to consider a vector $q = \dfrac{[\Omega, H]}{H^2}$ under condition of $(\Omega, H) = 0$.

Last condition necessary for $\Omega = [H, q]$ and checking of it is made similarly (only instead of vectors $\rho_k$ participate $[r_k, \rho_k]$), really:

$$(\Omega, H) = \frac{e}{\tau m_H c R^2} \sum_{k,l} (r_k, B)(r_l, B)(r_k, \rho_k, r_l) = \frac{e}{\tau m_H c R^2} \sum_{k<l} (r_k, B)(r_l, B)(r_k, \rho_k - \rho_l, r_l)$$

Continuation of equality with using $([r_k, \rho_k], r_k) = 0$ will be the following:

$$(\Omega, H) = \frac{e}{\tau m_H c R^2} \sum_{k<l} (r_k, B)(r_l, B)(([r_k, \rho_k], r_l) + ([r_l, \rho_l], r_k)) =$$

$$= \frac{e}{\tau m_H c R^2} \sum_k (r_k, B) r_k \sum_k (r_k, B)[r_k, \rho_k]$$

Performance of this condition too is reduced to the equation (3). Since this moment let's consider then after solution of equation (3) the vectors $r_k$ are replacing by $r_k^+ - r_0^+$ or $r_k^- - r_0^-$ (distinction of two this variant and definition of vectors $r_k^{\pm}$ situating on the line of moving of hydrogen atom will be explaining below).

The received expressions $M = [H, p]$ and $\Omega = [H, q]$ are necessary for pass to quantum - mechanical model that is to replace vectors by Hermit's operators (in this case matrixes), and vector multiplication – by the algebraic commutation. The quantum model is under construction by analogy to system of Hamilton where instead of Poisson's bracket is a commutation, and instead of moment of forces in the equation $M = [H, p] = \dot{p}$ is a time derivative of the moment of impulse (of the kinetic moment).

That is, if in the Cartesian right-orientation system of coordinates the components of vectors

$$H = \left(H_x, H_y, H_z\right); \; p = \frac{[M, H]}{H^2} = \left(p_x, p_y, p_z\right); \; q = \frac{[\Omega, H]}{H^2} = \left(q_x, q_y, q_z\right) \text{ are present, then equation of}$$

sublimer movement $\left(M_x, M_y, M_z\right) = \left(H_y p_z - H_z p_y, H_z p_x - H_x p_z, H_x p_y - H_y p_x\right)$ can be written down («$i$» - imaginary unit, $\overline{(\ldots)}$ - complex conjugation) as follows – right part of the following equality is a Hermit's matrixes commutation:
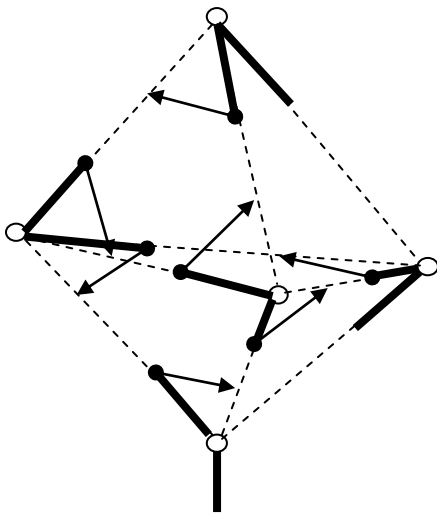


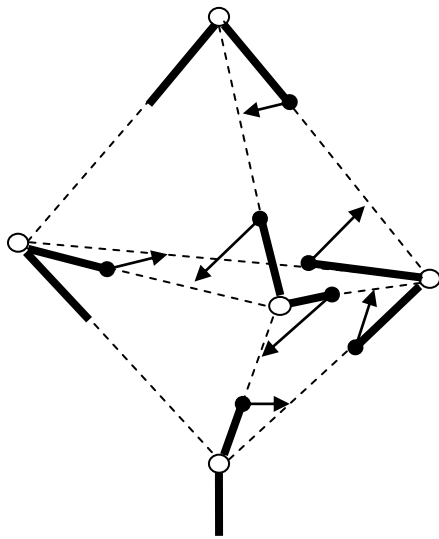**Figure 5.** State 5 and transition

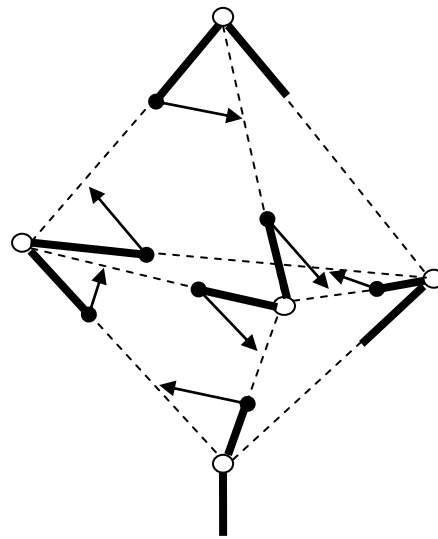$m = 5$ to state 4 ( $s = 3$ )
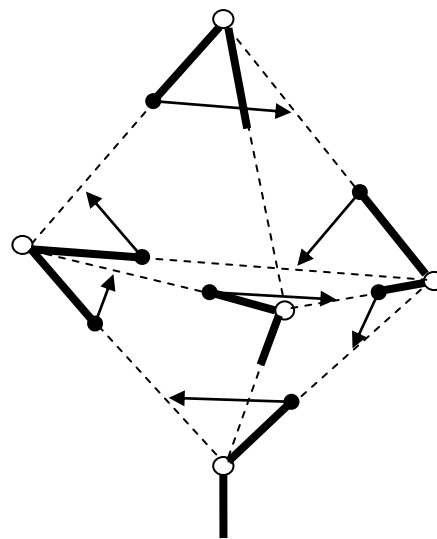


**Figure 6.** State 6 and transition

$m = 6$ to state 1 ( $s = 3$ )

**Figure 7.** Transition $m = 7$ between

states 4 and 6 ( $s = 3$ )



**Figure 8.** Transition $m = 8$ between

states 3 and 1 ( $s = 3$ )

$$\hat{q} = \begin{pmatrix} 0 & -iq_z & i\overline{q}_y \\ i\overline{q}_z & 0 & -iq_x \\ -iq_y & i\overline{q}_x & 0 \end{pmatrix} ; \quad \hat{p} = \begin{pmatrix} 0 & -ip_z & i\overline{p}_y \\ i\overline{p}_z & 0 & -ip_x \\ -ip_y & i\overline{p}_x & 0 \end{pmatrix} ; \quad \hat{H} = \begin{pmatrix} 0 & -iH_z & i\overline{H}_y \\ i\overline{H}_z & 0 & -iH_x \\ -iH_y & i\overline{H}_x & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & -M_z & M_y \\ M_z & 0 & -M_x \\ -M_y & M_x & 0 \end{pmatrix} = \begin{pmatrix} 0 & -ip_z & i\overline{p}_y \\ i\overline{p}_z & 0 & -ip_x \\ -ip_y & i\overline{p}_x & 0 \end{pmatrix} \begin{pmatrix} 0 & -iH_z & i\overline{H}_y \\ i\overline{H}_z & 0 & -iH_x \\ -iH_y & i\overline{H}_x & 0 \end{pmatrix} -$$

$$- \begin{pmatrix} 0 & -iH_z & i\overline{H}_y \\ i\overline{H}_z & 0 & -iH_x \\ -iH_y & i\overline{H}_x & 0 \end{pmatrix} \begin{pmatrix} 0 & -ip_z & i\overline{p}_y \\ i\overline{p}_z & 0 & -ip_x \\ -ip_y & i\overline{p}_x & 0 \end{pmatrix}$$

It is similarly possible to write down and the second equation of system of Hamilton's $\Omega = [H,q] = \dot{q}$ and using of quantum - mechanical analogy we consider a finite-dimension operators of physical values (matrixes of coordinates, impulse and hamiltonian):
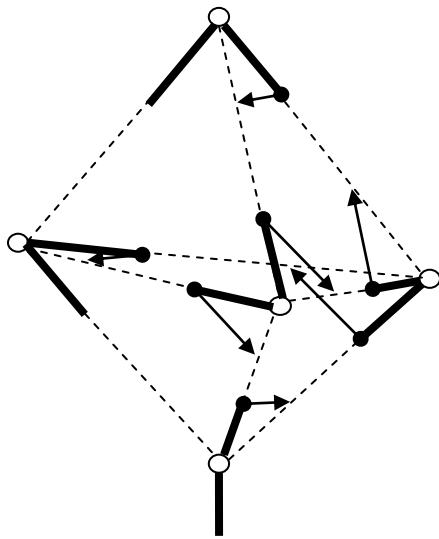
**Figure 9.** Transition $m = 9$ between

states 3 and 2 ($s = 3$)
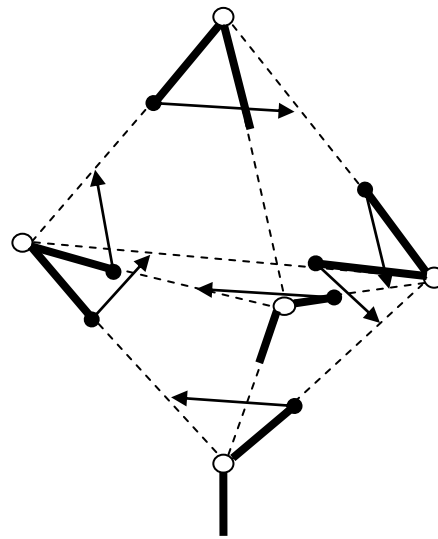


**Figure 10.** Transition $m = 10$ between

states 2 and 5 ($s = 3$)

Further it is possible to reduce a search problem of quantum levels and transitions between they for water sublimer to an algebraic kind.

$$\left|\hat{H} - \lambda E\right| = \begin{vmatrix} -\lambda & -iH_z & i\overline{H}_y \\ i\overline{H}_z & -\lambda & -iH_x \\ -iH_y & i\overline{H}_x & -\lambda \end{vmatrix} = -\lambda^3 + iH_x H_y H_z - i\overline{H}_x \overline{H}_y \overline{H}_z + \lambda\left(\left|H_x\right|^2 + \left|H_y\right|^2 + \left|H_z\right|^2\right) = 0$$

It is a cubic equation $\lambda^3 + \alpha\lambda + \beta = 0$ has a real roots at condition $\left(\dfrac{\alpha}{3}\right)^3 + \left(\dfrac{\beta}{2}\right)^2 < 0$, it's a following

from Hermit's properties of the matrix $\hat{H}$. Then the roots $\lambda = \lambda_1, \lambda_2, \lambda_3$ are

$$\lambda_1 = 2\sqrt{-\frac{\alpha}{3}}\cos\left(\frac{\gamma}{3} - \frac{2\pi}{3}\right), \lambda_2 = 2\sqrt{-\frac{\alpha}{3}}\cos\frac{\gamma}{3}, \lambda_3 = 2\sqrt{-\frac{\alpha}{3}}\cos\left(\frac{\gamma}{3} + \frac{2\pi}{3}\right) \quad \text{here} \quad \cos\gamma = \frac{-\beta}{2\sqrt{\left(-\frac{\alpha}{3}\right)^3}} \quad \text{and}$$

$\alpha = -\left|H_x\right|^2 - \left|H_y\right|^2 - \left|H_z\right|^2$, $\beta = 2\operatorname{Im}\left(H_x H_y H_z\right)$, $\operatorname{Im}$ – is imaginary part of complex number i.e. view of roots

$$\lambda_{1,2,3} = 2\sqrt{\frac{\left|H_x\right|^2 + \left|H_y\right|^2 + \left|H_z\right|^2}{3}}\cos\left(\frac{\gamma}{3} - \frac{2\pi}{3}, 0, +\frac{2\pi}{3}\right), \quad \cos\gamma = \frac{-\operatorname{Im}\left(H_x H_y H_z\right)}{\sqrt{\left(\dfrac{\left|H_x\right|^2 + \left|H_y\right|^2 + \left|H_z\right|^2}{3}\right)^3}}.$$

There are three quantum levels (three eigen-numbers of the hamiltonian matrix $l = 1, 2, 3$) according of are three eigen-vectors, the vectors are combining as orthogonal basis (in Hermit's sense)

$$\psi_l^m = \begin{pmatrix} -H_x^m H_z^m + i\lambda_l \overline{H}_y^m \\ -\overline{H}_y^m \overline{H}_z^m - i\lambda_l H_x^m \\ \lambda_l^2 - \left|H_z^m\right|^2 \end{pmatrix} \quad \text{for each of transitions } m = \pm 1, ..., \pm 15 \text{ i.e. for each } H^m.$$

Let's consider also distinction between two variants differing by values $r_0^+, r_0^-$ for which corresponding values $H_+^m, H_-^m$ are complex conjugated. We shall designate it as $H_\pm^m$ corresponding eigen-numbers $\lambda_{l\pm}^m$, values $q_\pm^m$ and eigen-vectors after normalization $\Psi_{l\pm}^m = \dfrac{\psi_{l\pm}^m}{\left\|\psi_{l\pm}^m\right\|}$. Let's attribute also probabilities $p_+ + p_- = 1$ of stay of sublimer in one of the qualities differing by values $r_0^+, r_0^-$, the physical sense of it will be explained further.

Now it is possible to consider $P_l^{nm} = \dfrac{p_+\left|\left(\Psi_{l+}^n, q_+^m\right)\right|^2 + p_-\left|\left(\Psi_{l-}^n, q_-^m\right)\right|^2}{\displaystyle\sum_{m(n)}\left(p_+\left|\left(\Psi_{l+}^n, q_+^m\right)\right|^2 + p_-\left|\left(\Psi_{l-}^n, q_-^m\right)\right|^2\right)}$ as probability of quantum transition with number «$m$» at a quantum level «$l$» provided that the previous transition had number «$n$», here $(,)$ and $\|...\|$ are Hermit's scalar multiplication and norm of vectors; the sum contains five terms corresponding five transitions possible of a state to which sublimer has come after transition «$n$».

One transition of type 1 is possible; two – type 2 and two types – 3 from any state. Set of possible transitions is conditional $m(n)$ and for each of states depend on numbering and further we will be certain by possible way of its doing. Stagnation during the time $\tau$ in the state is characterizing by probability $P_l^{nn}$. The probabilities which are not entering into set $m(n)$ are considered zero.
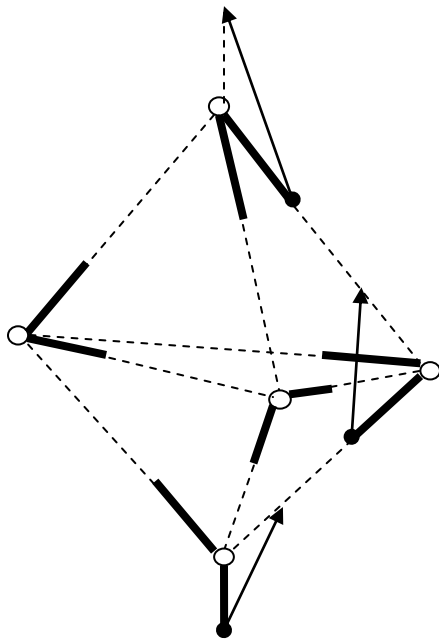
**Figure 11.** Change of orientation

of free hydrogen
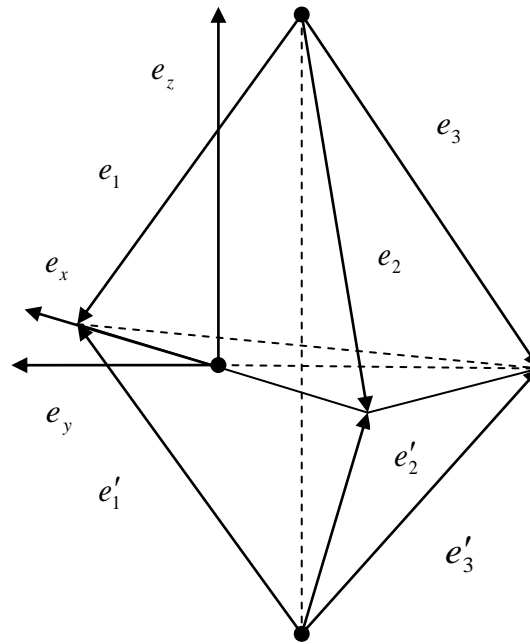


**Figure 12.** Systems of coordinates

connecting with water sublimer

For computation of $H$ (depending on transition) it is possible to connect with water sublimer the three systems of coordinates: the Cartesian system $(e_x, e_y, e_z)$ of right-orientations and two more auxiliary systems $(e_1, e_2, e_3)$ and $(e_1', e_2', e_3')$ – they are entered for convenience of transformations (fig. 12). Communication between vectors of last two auxiliary systems

$e_1' = e_1 - \dfrac{2}{3}(e_1 + e_2 + e_3)$ ; $e_2' = e_2 - \dfrac{2}{3}(e_1 + e_2 + e_3)$ ; $e_3' = e_3 - \dfrac{2}{3}(e_1 + e_2 + e_3)$ it is basis transformation

$$\begin{pmatrix} e_1' \\ e_2' \\ e_3' \end{pmatrix} = \frac{1}{3}\begin{pmatrix} 1 & -2 & -2 \\ -2 & 1 & -2 \\ -2 & -2 & 1 \end{pmatrix}\begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix} = A\begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix}$$ with matrix $A = A^* = A^{-1}$.

The vector $e_x$ has an identical direction with « $e_1 - e_2$ »; a vector $e_y$ - with « $\dfrac{1}{2}(e_1 + e_2) - e_3$ »; a vector $e_z$ - with « $-(e_1 + e_2 + e_3)$ ». Including that and the vectors of all basis have unit length and skeleton of the water sublimer consists of two tetrahedrons we use scalar multiplications $(e_1, e_2) = (e_2, e_3) = (e_3, e_1) = \dfrac{1}{2}$ then:

$$e_x = e_1 - e_2 \; ; \; e_y = \frac{1}{\sqrt{3}}(e_1 + e_2 - 2e_3) \; ; \; e_z = \frac{1}{\sqrt{6}}(e_1 + e_2 + e_3)$$

Further we shall consider two vectors $r_+, r_-$ are having beginning points in the geometrical center of sublimer skeleton but ending ones in two symmetric tops (on fig. 12 they are up and down tops accordingly):

$$r_+ = -\frac{1}{3}(e_1 + e_2 + e_3) = -r_- = \frac{1}{3}(e_1' + e_2' + e_3') \text{ then } e_1' - e_1 = e_2' - e_2 = e_3' - e_3 = r_+ - r_-$$

Also we shall consider three vectors initial from center of sublimer with final points in its three tops located on a plane of symmetry.

$$r_a = r_+ + e_1 = r_- + e_1' = \frac{1}{3}(2e_1 - e_2 - e_3) = \frac{1}{3}(2e_1' - e_2' - e_3') \; ;$$

$$r_b = r_+ + e_2 = r_- + e_2' = \frac{1}{3}(-e_1 + 2e_2 - e_3) = \frac{1}{3}(-e_1' + 2e_2' - e_3') \; ;$$

$$r_c = r_+ + e_3 = r_- + e_3' = \frac{1}{3}(-e_1 - e_2 + 2e_3) = \frac{1}{3}(-e_1' - e_2' + 2e_3') \text{ then}$$

$$e_1 - e_2 = e_1' - e_2' = r_a - r_b \; ; \; e_2 - e_3 = e_2' - e_3' = r_b - r_c \; ; \; e_3 - e_1 = e_3' - e_1' = r_c - r_a .$$

By means of these vectors it is possible to express vectors of displacement of atoms of hydrogen $\rho_k$ and also to define radius-vectors $r_k$ initial from geometrical center of sublimer skeleton and finals is average points of vectors $\rho_k$. Further it is necessary to satisfy conditions $(\rho_k, r_k) = 0$ and (3) by change of initial and final points of vectors $r_k$ but with keeping a straight line passing through a point $r_k$ with direction vector $\rho_k$ – a line of movement of atom of hydrogen.

For this purpose we can copy conditions in the form of $(\rho_k, r_k^\pm - r_0^\pm) = 0$ for searching the points $r_k^+$ or $r_k^-$ in complex space then $r_k^\pm = r_k - \dfrac{(r_k - r_0^\pm, \rho_k)}{\|\rho_k\|^2}\rho_k$ here the scalar multiplication and norm Euclid's type are present. Solution of the equation (3) i.e. searching of $r_0^\pm$ is make in the system of coordinates with a basis $(e_x, e_y, e_z)$ located in the geometrical center of sublimer skeleton, coordinates of vectors $r_k$ in the equation (3) will be specified below. After it shall done the vectors $r_k$ exchange by $r_k^\pm - r_0^\pm$ is make in all formulas.

It is possible to make scaling: if accept as unit length of an edge the sublimer $R$ instead of physical values $r_k^\pm - r_0^\pm$ we consider $\left(r_k^\pm - r_0^\pm\right)R$, here $r_k^\pm - r_0^\pm$ already dimensionless then expressions (2, 4) will become:

$$H_\pm^n = \frac{e}{m_H c}\sum_k \left(r_k^\pm - r_0^\pm, B\right)\left(r_k^\pm - r_0^\pm\right); \quad \Omega_\pm^n = \frac{e}{m_H c}\sum_k \left(r_k^\pm - r_0^\pm, B\right)\left[r_k^\pm - r_0^\pm, q_k\right].$$ If instead of an induction

$B$ we consider vector of direction $b = \dfrac{B}{|B|}$ then

$$H_\pm^n = \frac{1}{\tau}\sum_k \left(r_k^\pm - r_0^\pm, b\right)\left(r_k^\pm - r_0^\pm\right); \quad \Omega_\pm^n = \frac{1}{\tau}\sum_k \left(r_k^\pm - r_0^\pm, b\right)\left[r_k^\pm - r_0^\pm, q_k\right] \qquad (5)$$

from physical sizes there will be only a time scale $\tau$.

If to consider the time a continuous instead of discrete as in a considered case then classical quantum-mechanical theory gives commutation of times derivative and spatial averaging of physical values under condition of performance of Schrödinger's equation: $i\dfrac{\partial \psi}{\partial t} = \hat{H}\psi$; $\hat{H}$ – a hamiltonian operator; $\psi(t)$ – a wave function represented by decomposition $\psi = \sum_l A_l \psi_l \exp\left(-i\dfrac{\lambda_l}{\tau}t\right)$ using the eigen-functions of hamiltonian operator $\tau \hat{H}\psi_l = \lambda_l \psi_l$.

In reality for dimer of water $R \approx 0.294\, nm$ and distance between atoms of oxygen and hydrogen in water molecule $r \approx 0.099\, nm$ therefore after the scaling is possible to consider this distance as dimensionless value $\rho = \dfrac{r}{R} \approx 0.3367$. After that it is possible to express dimensionless vectors $r_k$ and $\rho_k$ through basic vectors $\left(e_x, e_y, e_z\right)$ or auxiliary vectors $\left(e_1, e_2, e_3\right)$ and $\left(e_1', e_2', e_3'\right)$.

So, for transition $m = 1$ between states 1 - 4 (fig. 1) $N = 4$ – number of hydrogen atoms moving with connections;

$$r_1 = r_+ + \frac{\rho}{2}\left(e_1 + e_2\right); \; \rho_1 = \rho\left(e_1 - e_2\right); \; r_2 = r_a - \frac{\rho}{2}\left(e_1 + e_1'\right); \; \rho_2 = \rho\left(e_1 - e_1'\right);$$

$$r_3 = r_b - \frac{\rho}{2}\left(e_2 + e_2'\right); \; \rho_3 = \rho\left(e_2' - e_2\right); \; r_4 = r_- + \frac{\rho}{2}\left(e_1' + e_2'\right); \; \rho_4 = \rho\left(e_2' - e_1'\right);$$

for transition $m = 3$ between states 3 - 6 (fig. 3) $N = 4$ ;

$$r_1 = r_+ + \frac{\rho}{2}(e_2 + e_3); \ \rho_1 = \rho(e_2 - e_3) \ ; \ r_2 = r_b - \frac{\rho}{2}(e_2 + e_2'); \ \rho_2 = \rho(e_2 - e_2') \ ;$$

$$r_3 = r_c - \frac{\rho}{2}(e_3 + e_3'); \ \rho_3 = \rho(e_3' - e_3) \ ; \ r_4 = r_- + \frac{\rho}{2}(e_2' + e_3'); \ \rho_4 = \rho(e_3' - e_2') \ ;$$

for transition $m = 4$ between states 4 - 3 (fig. 4) $N = 3$ ;

$$r_1 = r_a + \frac{\rho}{2}(e_2 + e_3 - 2e_1); \ \rho_1 = \rho(e_3 - e_2) \ ; \ r_2 = r_b + \frac{\rho}{2}(e_1 + e_3 - 2e_2); \ \rho_2 = \rho(e_1 - e_3) \ ;$$

$$r_3 = r_c + \frac{\rho}{2}(e_1 + e_2 - 2e_3); \ \rho_3 = \rho(e_2 - e_1) \ ;$$

for transition $m = 5$ between states 5 - 4 (fig. 5) $N = 7$ ;

$$r_1 = r_+ + \frac{\rho}{2}(e_1 + e_2); \ \rho_1 = \rho(e_1 - e_2) \ ; \ r_2 = r_a + \frac{\rho}{2}(e_2 - 2e_1); \ \rho_2 = \rho e_2 \ ;$$

$$r_3 = r_a + \frac{\rho}{2}(e_3' - 2e_1'); \ \rho_3 = -\rho e_3' \ ; \ r_4 = r_b + \frac{\rho}{2}(e_1 - 2e_2); \ \rho_4 = -\rho e_1 \ ;$$

$$r_5 = r_b + \frac{\rho}{2}(e_3' - 2e_2'); \ \rho_5 = \rho e_3' \ ; \ r_6 = r_c + \frac{\rho}{2}(e_1 + e_2 - 2e_3); \ \rho_6 = \rho(e_1 - e_2) \ ;$$

$$r_7 = r_- + \frac{\rho}{2}(e_1' + e_2'); \ \rho_7 = \rho(e_2' - e_1') \ ;$$

for transition $m = 7$ between states 4 - 6 (fig. 7) $N = 7$ ;

$$r_1 = r_+ + \frac{\rho}{2}(e_2 + e_3); \ \rho_1 = \rho(e_2 - e_3) \ ; \ r_2 = r_b + \frac{\rho}{2}(e_1 - 2e_2); \ \rho_2 = \rho e_1 \ ;$$

$$r_3 = r_b + \frac{\rho}{2}(e_3' - 2e_2'); \ \rho_3 = -\rho e_3' \ ; \ r_4 = r_c + \frac{\rho}{2}(e_1 - 2e_3); \ \rho_4 = -\rho e_1 \ ;$$

$$r_5 = r_c + \frac{\rho}{2}(e_2' - 2e_3'); \ \rho_5 = \rho e_2' \ ; \ r_6 = r_a + \frac{\rho}{2}(e_2 + e_3 - 2e_1); \ \rho_6 = \rho(e_3 - e_2) \ ;$$

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$$r_7 = r_- + \frac{\rho}{2}\left(e_2' + e_3'\right); \; \rho_7 = \rho\left(e_3' - e_2'\right).$$

Numeration of states and all transitions between them can be any, if « $m$ » is number of transition between states « $j_k^1, j_k^2$ » then « $-m$ » is a return transition « $j_k^2, j_k^1$ ». In figures it corresponds to change of $\rho_k$ signs and displacement of hydrogen atoms along arrows to the opposite ends of vectors $\rho_k$.

We shall consider group of symmetry in set of sublimer motion for proving the fact of it's a five-dimensional tetrahedron. Let's consider cyclic rearrangements of indexes $1 \rightarrow 2 \rightarrow 3 \rightarrow 1$ and $a \rightarrow b \rightarrow c \rightarrow a$ in the right parts of equations of $r_k, \rho_k$, they are correspond to turns of sublimer skeleton around of a vertical axis. If at one such rearrangement the state of sublimer and transition from it with number « $m$ » is turned to other state and transition « $n$ » (the vectors $\rho_k$ and all hydrogen communications are coincides) it we shall designate as « $m_+ = n$ » or the same « $m = n_-$ » (the index minus designates cyclic rearrangement and turn in the opposite direction - inverse). The two equations are equivalent with such $m_- = n_+$.

Let's notice for example $1_- = 2$ but $2_- \neq 3 \neq 1_+$ and $4 \neq 4_+$ (see figs. $1-4$; designation $\neq$ means that not all hydrogen communications coincides). The set of transitions thus is algebraic group with composition as operation.

It is possible to choose the minimal subset of transitions which at the specified cyclic rearrangements act on all set (all 15 transitions become covered) if direct and return transitions are identified. The choice of this minimal subset is ambiguous, and it can be made by following way.

It is possible to write out all chains of the equations received at cyclic rearrangements of indexes (at rotations of sublimer around of a vertical axis) and write out all transitions not included to chains. Numeration of states on figs. $1-10$ correspond the chains $1_- = 2 ; 3 ; 4 ; 5_- = 6 = 9_+ ; 7 = -8_+ = 10_-$. Thus any of equation of one chain should not follow from equations of others chains and in presented set of five chains two are complete but three are uncompleted. If addition of other transitions any more does not lead to occurrence of new chains (the full chain consists of three transitions and each transition is included only into one chain) then minimal set consists of "representatives" – by one transition from each chain and it is necessary condition for structure of the minimal set of transitions. Choosing numeration give for example $1, 3, 4, 5, 7$ is minimal set of transitions.

At two consecutive cyclic rearrangements the minimal set of five transitions (they are resulted above as formulas for $r_k, \rho_k$) will give in addition ten new transitions, and it in the sum will make all set of the transitions corresponding of edges of a five-dimensional tetrahedron of states of water sublimer. Possible proving that the five

full chains of equations consist from two chains of transitions type 3, two chains of transitions type 2 and one chain of transitions type 1 – they are corresponds to edges of tetrahedron of states issuing from one top (from one state of sublimer) is not present.

## Results and Discussion

The purpose of construction of mathematical model is extraction of the deterministic component in behavior of water sublimer under action of a homogeneous and constant magnetic field (formalization which will allow to explain that dynamics of sublimer in such conditions is not absolutely chaotic process). So 6 states of water sublimer and 30 transitions are described in the model by considered probabilities $P_l^{nm}$. What is necessary to add for full description of sublimer dynamics i.e. for computations of probabilities $P_l^{nm}$, otherwise, than behavior of water sublimer at movement differs from usual Markov's process? In usual autonomic Markov's process there is no concept of quantum levels, but in our case it is necessary to add dependence on a quantum level and if to consider this dependence determined (not casual) it can be made as follows: real eigen-numbers $\lambda_{1\pm}^m, \lambda_{2\pm}^m, \lambda_{3\pm}^m$ are situate in ascending order (for each of variants « $\pm$ ») and singular cases of conterminous roots are not considered, thus on indexes of roots $\lambda_{\sigma(1\pm)}^m, \lambda_{\sigma(2\pm)}^m, \lambda_{\sigma(3\pm)}^m$ rearrangement $\sigma_m$ is make.

The hypothesis about partially deterministic behavior of water sublimer consists in the assumption of following dependence between a quantum level (on which was made a transition with number « $m$ ») and of the transition type $s = \sigma_m(l)$. There is still an ambiguity of the choice $r_0^+, r_0^-$, described by probabilities $p_+, p_-$ which is presumably connected with orientation of "free" hydrogen. This orientation for all sublimers of a ideal chain of water, should be identical (differently the chain will be broken off) and depends on conditions on the ends of a chain. Thus, the probabilities setting orientation of "free" hydrogen, satisfying to a condition $p_+ + p_- = 1$, can be considered as external data (not dependent on internal dynamics of sublimer).

## Conclusion

The constructed mathematical model meets following requirements. It describes quantum transitions between states of water sublimer, as result of actions of a magnetic field. Accordingly and quantum levels are directly connected with a magnetic induction. Modeling the sublimer of water i.e. of dynamics of discrete behavior, in particular, allow to calculate the probabilities of transition between its states in dependence with quantum levels (energy source is a magnetic field but communication conditions are rules Bernal – Fowler, constants of interaction potential and condition of an invariance of sublimer position in chained structure of water).

The basic assumption of the model is a angular values between hydrogen communications in four molecules of water sublimer are equal $\pi/3$ also preservation of position of sublimer concerning power lines of a

magnetic field and orientation of free hydrogen. There is a question of physical correctness of the assumptions. In amorphous structure of water such state is impossible however is possible to present a situation which is hypothetically in view of nano-technologies development. Namely, we shall present such chain of water sublimers, concluded inside of carbon nano-pipe. Diameter of such pipe has the size nearby 0.6 nm, the size of sublimer crossing by plane of its symmetry nearby 0.3 nm.

Proceeding from the general reasons, and according to the equations of the presented mathematical model, characteristic time of inwardness change of the sublimer has the order $\tau = \dfrac{m_H c}{e|B|}$. It is $\tau \approx 10^{-8} s$ in average magnetic fields (the order 1 *T*) and it is much more than «time of a life» of the molecules in amorphous structure of water. Hence, physical properties of such nano-material in a magnetic field can be rather interesting and it may be used for production of it. Experiments specify that action of Lorenz forces on molecular communications of water (at long time magnetic treatment [2]) render the essential influence on the properties.

The basic attribute of the presented model it's describing only three quantum levels of water sublimer. It can be coordinated with available experimental data only qualitatively in view of hypothetically such water structure. So, in work [3] results of measurement of electro-kinetic $\varsigma$-potential with an impurity of $CaCO_3$ at X-ray diffraction for usual and magneto-treatment waters are presented. As a result essential differences of molecular-energy characteristics for usual and magneto-treatment waters are found out and in the diagrams of diffraction three new splashes are appear after magneto-treatments. However in amorphous and crystal structures of water the magnetic field action can not have so much changing of properties because the structure is not exactly periodic. One – dimensional periodicity (like for the discussed hypothetically) it is the more suitable case for it.

## References

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