

A Fiber Bundle Model of the Ice I_h Structure

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Abstract

A three-dimensional model of ice I_h based on the fiber bundle approach is presented. A hybrid structure of ice consisting of the oxygen lattice with the $P6_3/mmc$ crystallographic symmetry and the hydrogen subsystem satisfying the Bernal-Fowler rules is considered. Controllable change of the protons position at hydrogen bounds by optoacoustic perturbation is discussed. Both classic and bispinor Hamiltonians are proposed.

Forecasting intensive progress in microphysics as early as in 1959, R. Feynman has made a presentation at the annual session of the American Physical Society under the symbolic title "There's plenty of room at the bottom" [1]. He underlined that microcosm can give in future practically unlimited possibilities for material technology and information processing. But for achievement of practical results, it is necessary to overcome not a few obstacles. And one of them is the gap between micro- and macrolevels which prevents a direct contact without information losses and order distraction. Over the year, it was clearly understood that control and information theory should play an important role in microphysics progress as well as in molecular and quantum computing [2–7]. First of all, proper modelling of hybrid systems must be developed. One of possible models is presented here.

Hexagonal ice I_h was chosen as an object thanks to its wide spread in nature and because it allows information processing at the molecular level. We start from the brief description of the usual ice structure following the short but very consistent book of N. Maeno [8]. Hexagonal modification of ice exists under normal pressure and temperature $T < -6$ °C. It has the crystallographic symmetry $P6_3/mmc$ but only for the oxygen lattice, the hydrogen subsystem is characterized by relative arbitrariness in protons' distribution at hydrogen bonds. So if the Bernal-Fowler rules are fulfilled, the protons have many variants of distribution. These rules are the next:

- 1) exactly two protons are situated beside every oxygen atom,
- 2) exactly one proton is present at every hydrogen bond.

Mathematically, they can be expressed with some equations binding binary variables for bistable proton positions at hydrogen bonds. This and another technique will be demonstrated below.

One of possible dispositions of protons in the frame of an ice I_h elementary cell is shown in Fig.1. Framework of the cell is composed of two mirror symmetric strata which are based on local orthogonal triplets $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ (lower, right) and $\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3$ (upper, left) with the origins situated at the endpoints of the vertical hydrogen bond. The triplets are oriented towards middle points of tetrahedron edges which are connected with the

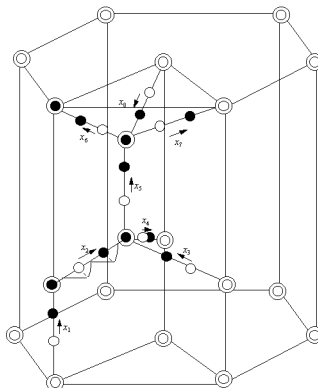


Fig.1.

correspondent oxygen atoms. Hydrogen bonds geometrically are represented by vectors $\mathbf{f}_i, \mathbf{f}'_i$ ($i = 0, 1, 2, 3$), so that

$$\begin{aligned} \mathbf{e}_1 &= \frac{1}{2}(\mathbf{f}_1 + \mathbf{f}_0), & \mathbf{e}_2 &= \frac{1}{2}(\mathbf{f}_2 + \mathbf{f}_0), & \mathbf{e}_3 &= \frac{1}{2}(\mathbf{f}_3 + \mathbf{f}_0); \\ \mathbf{e}'_1 &= -\frac{1}{2}(\mathbf{f}'_1 + \mathbf{f}'_0), & \mathbf{e}'_2 &= -\frac{1}{2}(\mathbf{f}'_2 + \mathbf{f}'_0), & \mathbf{e}'_3 &= -\frac{1}{2}(\mathbf{f}'_3 + \mathbf{f}'_0); \\ \mathbf{f}_0 + \mathbf{f}_1 + \mathbf{f}_2 + \mathbf{f}_3 &= 0, & \mathbf{f}'_0 + \mathbf{f}'_1 + \mathbf{f}'_2 + \mathbf{f}'_3 &= 0; \\ \mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3 &= \mathbf{f}_0 = \mathbf{f}'_0 = -(\mathbf{e}'_1 + \mathbf{e}'_2 + \mathbf{e}'_3); \\ \mathbf{f}_1 &= \mathbf{e}_1 - \mathbf{e}_2 - \mathbf{e}_3, & \mathbf{f}_2 &= -\mathbf{e}_1 + \mathbf{e}_2 - \mathbf{e}_3, & \mathbf{f}_3 &= -\mathbf{e}_1 - \mathbf{e}_2 + \mathbf{e}_3; \\ \mathbf{f}'_1 &= -(\mathbf{e}'_1 - \mathbf{e}'_2 - \mathbf{e}'_3) = -\frac{5}{3}\mathbf{e}_1 + \frac{1}{3}\mathbf{e}_2 + \frac{1}{3}\mathbf{e}_3 = -\left(\mathbf{f}_1 + \frac{2}{3}\mathbf{f}_0\right), \\ \mathbf{f}'_2 &= -(-\mathbf{e}'_1 + \mathbf{e}'_2 - \mathbf{e}'_3) = \frac{1}{3}\mathbf{e}_1 - \frac{5}{3}\mathbf{e}_2 + \frac{1}{3}\mathbf{e}_3 = -\left(\mathbf{f}_2 + \frac{2}{3}\mathbf{f}_0\right), \\ \mathbf{f}'_3 &= -(-\mathbf{e}'_1 - \mathbf{e}'_2 + \mathbf{e}'_3) = \frac{1}{3}\mathbf{e}_1 + \frac{1}{3}\mathbf{e}_2 - \frac{5}{3}\mathbf{e}_3 = -\left(\mathbf{f}_3 + \frac{2}{3}\mathbf{f}_0\right). \end{aligned}$$

Following the relations between vectors and having used the length of hydrogen bonds

$$d = |\mathbf{f}_i| = |\mathbf{f}'_i| = 0.276 \text{ nm}, \quad (i = 0, 1, 2, 3)$$

one can determine horizontal a and vertical h moduli of the hexagonal lattice:

$$a = |\mathbf{f}_2 - \mathbf{f}_3| = |\mathbf{a}_1| = |\mathbf{f}_3 - \mathbf{f}_1| = |\mathbf{a}_2| = \frac{2}{3}\sqrt{6}d = 0.452 \text{ nm},$$

$$h = |\mathbf{a}_3| = |2\mathbf{f}_0 - \mathbf{f}_3 - \mathbf{f}'_3| = \frac{8}{3}d = 0.736 \text{ nm}.$$

Proton configuration can be specified by different methods. One of them was applied in [6] to cubic ice I_c where protons' positions have been determined by binary variables $z_\alpha(\mathbf{n}) \in GF(2)$ ($\alpha = 0, 1, 2, 3; \mathbf{n} \in Z^3$). Displacement of protons from middles of hydrogen bonds could be expressed as follows:

$$x_\alpha(\mathbf{n}) = \frac{1}{2}(-1)^{z_\alpha(\mathbf{n})} = \pm \frac{1}{2}.$$

It was found that the Bernal-Fowler rules could be written in the form of homogenous equations

$$\sum_{\alpha=0}^3 x_{\alpha}(\mathbf{n}) = 0, \quad \sum_{\alpha=0}^3 x_{\alpha}(\mathbf{n} + \mathbf{e}_{\alpha}) = 0 \quad (\mathbf{n} \in Z^3),$$

where $\mathbf{e}_0 = \{0, 0, 0\}$, $\mathbf{e}_1 = \{1, 0, 0\}$, $\mathbf{e}_2 = \{0, 1, 0\}$, $\mathbf{e}_3 = \{0, 0, 1\}$.

These equations are linear relatively to $x_{\alpha}(\mathbf{n})$ but not to $z_{\alpha}(\mathbf{n})$. So definite selection rules should be applied after all. This hidden nonlinearity becomes explicit when another method is attracted.

Beforehand, let us make some notifications:

- near every node of the oxygen lattice, exactly 1 pair of protons can be found which may occupy 4 hydrogen bonds (outcoming from the given node) by $C_4^2 = 6$ different possible variants;

- hydrogen dihedron $D_{\alpha}(\mathbf{n})$ (α - node's number, \mathbf{n} - elementary cell number) formed by two unitary vectors $\mathbf{r}_{\alpha}^{(1)}(\mathbf{n})$, $\mathbf{r}_{\alpha}^{(2)}(\mathbf{n})$ directed from the oxygen node to protons remains scalar product $\langle \mathbf{r}_{\alpha}^{(1)}(\mathbf{n}), \mathbf{r}_{\alpha}^{(2)}(\mathbf{n}) \rangle = \text{const}$ in all 6 possible positions of its bisectrix unitary vector $\mathbf{d}_{\alpha}(\mathbf{n}) = \frac{\sqrt{3}}{2} [\mathbf{r}_{\alpha}^{(1)}(\mathbf{n}) + \mathbf{r}_{\alpha}^{(2)}(\mathbf{n})]$;

- dihedron bisectrix unitary vector $\mathbf{d}_{\alpha}(\mathbf{n})$ can be oriented at every vertex of an octahedron inscribed in the tetrahedron surrounding a given node of the lattice if this is not forbidden by neighboring dihedron positions;

- dihedron's position is identically determined by the index $\lambda_{\alpha}(\mathbf{n}) = 0, 1, \dots, 5$ of vector's $\mathbf{d}_{\alpha}(\mathbf{n})$ projection on the horizontal plane.

Let us introduce in residue class ring Z_6 characteristic functions for some of its subsets:

$$\begin{aligned} \Phi(\lambda_{\alpha}) &= \begin{cases} 0 & (\lambda = 5, 0, 1) \\ 1 & (\lambda = 2, 3, 4) \end{cases} = \begin{cases} 0 & \text{when } |\lambda| \leq 1 \pmod{6} \\ 1 & \text{when } |\lambda| > 1 \pmod{6} \end{cases} = \\ &= \{\lambda \pmod{2} + [\lambda \pmod{3}]^2 \pmod{2}\}; \\ \Theta(\lambda_{\alpha}) &= \begin{cases} 0 & (\lambda = 0, 2, 4) \\ 1 & (\lambda = 1, 3, 5) \end{cases} = \lambda \pmod{2}; \\ \Phi^+(\lambda_{\alpha}) &= \Phi(\lambda_{\alpha} + 2), \quad \Phi^-(\lambda_{\alpha}) = \Phi(\lambda_{\alpha} - 2). \end{aligned} \tag{1}$$

Now the Bernal-Fowler rules have an explicitly nonlinear character as follows:

$$\begin{aligned} \Phi[\lambda_1(\mathbf{n})] - \Phi[\lambda_2(\mathbf{n})] &= 0, \\ \Phi^+[\lambda_1(\mathbf{n} - \nu_1)] - \Phi^+[\lambda_2(\mathbf{n})] &= 0, \\ \Phi^-[\lambda_1(\mathbf{n})] - \Phi^-[\lambda_2(\mathbf{n} - \nu_2)] &= 0, \\ \Theta[\lambda_1(\mathbf{n} - \nu_3)] + \Theta[\lambda_2(\mathbf{n})] &= 0. \end{aligned} \tag{2}$$

Here, $\nu_1 = \{1, 0, 0\}$, $\nu_2 = \{0, 1, 0\}$, $-\nu_3 = \{0, 0, 1\}$, $\mathbf{n} = \{n_1, n_2, n_3\}$ ($\nu_1, \nu_2, \nu_3, \mathbf{n} \in Z_{N_1} \times Z_{N_2} \times Z_{N_3} \subset Z^3$), $\lambda_1(\mathbf{n})$ corresponds to the lower end of a sloping hydrogen bond and $\lambda_2(\mathbf{n})$ - to upper one. Every solution of this system conforms to set of mutually crossing contours covering the whole oxygen lattice - so-called Bernal-Fowler fibers oriented in accordance with protons' shifts.

There is no possibility to find a general solution of system (2) because unknown variables are determined in the ring which has zero divisors 2 and 3. (In this ring, $2 \times 3 = 6 = 0 \pmod{6}$.) Although the number of Diophantine equations in system (2) is twice that of unknowns, its solution exists. For example, $\lambda_1(n_1, n_2, n_3) = \lambda_2(n'_1, n'_2, n'_3) = \lambda_2(n_1, n_2, n_3 + 1) + 3 \pmod{6}$. Quantity of solutions is rapidly growing with the numbers N_1, N_2, N_3 . As an alternative to unknowns λ_i , one may choose pairs of unknowns $\sigma_i = \lambda_i \pmod{2}$ and $\mu_i = \lambda_i \pmod{3}$ which have been mentioned in (1). Their totality precisely corresponds to the number of equations (2) but, regrettably, two-moduli arithmetics appears in this case.

So it remains to take advantage of the recurrent procedure for finding solutions. For the clear presentation, each fragment (lower or upper) of the elementary cell can be imaged as a 6-pole $\Pi(\mathbf{n})$. Let us code an input $\mathbf{x} = \{x_1, x_2, x_3\}$ and outputs $\mathbf{x}' = \{x'_1, x'_2, x'_3\} = \{x'_1(\mathbf{n} - \nu_1), x'_2(\mathbf{n} - \nu_2), x'_3(\mathbf{n} - \nu_3)\}$ by binary integers from the ring Z_2 . For shifts X, Y, Z which can be ± 1 , it immediately follows

$$X = (-1)^{x_1}, \quad (-Y) = (-1)^{x_2}, \quad Z = (-1)^{x_3}$$

corresponding to the second ice rule:

$$X^2 = Y^2 = Z^2 = (-1)^{2x_i} = 1 \quad (i = 1, 2, 3).$$

Meanwhile making use of the first ice rule, one can obtain for the $\Pi(\mathbf{n})$ three-sheeted mapping

$$\Pi : Z_2^3 = Z_2 \times Z_2 \times Z_2 \rightarrow Z_2,$$

$$x'_i = \pi_i^\mu(x) \quad (0 = 1, 2, 3; \quad 1 \leq \mu \leq m(x) \leq 3)$$

which is represented in Table 1.

Table 1

N	x	π_i^1	π_i^2	π_i^3	$m(x)$
0	000	000	—	—	1
1	100	100	010	001	3
2	010	100	001	—	2
3	110	110	101	011	3
4	001	100	010	001	3
5	101	110	011	—	2
6	011	110	101	011	3
7	111	111	—	—	1

Apparently, the total number of different sorts of transformation is $2^2 \times 3^4 = 324$, but when x is fixed, $m(x) \leq 3$. By the way, it is easy to calculate the total amount of variants for the protons' distribution in one half-cell as the sum of all possible $m(x)$: $2 + 2 \times 2 + 4 \times 3 = 18$.

The algorithm is being built in the following manner. For a given rectangular parallelepiped P having $S_1 \times S_2 \times S_3$ layers in three orthogonal directions in the basis

$$\mathbf{b}_1 = \frac{1}{2}(\mathbf{a}_1 + \mathbf{a}_2), \quad \mathbf{b}_2 = \mathbf{a}_1 - \mathbf{a}_2, \quad \mathbf{b}_3 = \mathbf{a}_3,$$

one can fix definite mappings from Table 1 for all half-cells of P. Boundary conditions must be determined for 4 its bounds: 1 face, 2 sides and 1 lower:

$$\begin{aligned} x(s) \Big|_{s_1=0} &= X_1(s_2, s_3), & x(s) \Big|_{s_2=0} &= X_2^{(0)}(s_1, s_3), \\ x(s) \Big|_{s_2=s_2-1} &= X_2^{(1)}(s_1, s_3), & x(s) \Big|_{s_3=0} &= X_3(s_1, s_2). \end{aligned}$$

Because all half-cells in each layer are chess-ordered in the basis $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$, their inputs are fully independent in every row. Thereby, a complete decomposition of vertical columns is assured and wide parallelizing of output calculations is achieved for all layers. When the mapping distribution is fixed, there is possible to realize $2^{2S_3} + 1$ states with various inputs x, y, z in each column. In its turn, provided inputs are given in one column, one can obtain not more than 3^{S_3} states because, in every half-cell, maximum 3 mappings can be permitted. So the upper limit of the possible states quantity in a column is $2^{2S_3+1} \times 3^{S_3}$, and respectively, for a whole parallelepiped P with dimensions $S_1 \times S_2 \times S_3$ (in half-cell units) the upper limit of the possible states number is determined as

$$M = 2^{S_1 S_2 (2S_3+1)} \times 3^{S_1 S_2 S_3}.$$

If bonds between half-cells are ignored, each of them gives 2×3^2 combinations of protons' distributions as have been mentioned above. For $S_1 \times S_2 \times S_3$ half-cells, it turns out that the upper limit of the states number in this case is

$$M_0 = 2^{S_1 S_2 S_3} \times 3^{2S_1 S_2 S_3}.$$

Comparison M_0 with M shows that, when $S_3 \gg 1$, bonding between half-cells sufficiently decreases the quantity of possible configurations for the proton subsystem. As can be seen directly, the proposed algorithm is exhausting and does not give repetitions of variants.

Now the protons' subsystem information entropy S can be estimated:

$$S \leq \log_2 M = S_1 S_2 S_3 \left[\log_2 3 + 2 \left(1 + \frac{1}{2S_3} \right) \right].$$

Hence, specific entropy per one half-cell has the upper limit as follows:

$$S \leq \lim_{S_1 \rightarrow \infty} \lim_{S_2 \rightarrow \infty} \lim_{S_3 \rightarrow \infty} \frac{\log_2 M}{S_1 S_2 S_3} = 2 + \log_2 3 \simeq 3,6.$$

Without bounding between half-cells, specific entropy is found to be noticeably greater:

$$S_0 = \lim_{S_1 \rightarrow \infty} \lim_{S_2 \rightarrow \infty} \lim_{S_3 \rightarrow \infty} \frac{\log_2 M}{S_1 S_2 S_3} = 1 + 2 \log_2 3 \simeq 4,2.$$

A control problem for the hydrogen subsystem consists in determining and realization of a necessary sequence in the state space of all possible protons configurations. One can consider this sequence as a one-parameter subgroup of the structural group G of a fiber bundle (X_F, P_F^t, B, F) with the orbit space $X_F = (X \times F)/G \xrightarrow{P_F^t} B$ where the base B and layer F are the state space of protons and cotangent space, respectively. From physical viewpoint, it must be required to satisfy the stability of mapping in order to secure information processing from the destruction caused by dynamic chaotization.

Controlling action on the proton subsystem from the oxygen lattice deformations is effected by variations of the potential function. As this takes place, excitation is supposed

not so much to cause ionizing effects and proton transport but sufficient for displacements of protons along hydrogen bonds where they are situated. Electron shell deformations will be considered as adiabatic. Taking into account all these conditions, let us construct such a nonstationary Hamiltonian that can be decomposed by a periodically time-dependent orthogonal canonical transformation into a direct sum of Hamiltonians for bistable nonlinear oscillators. Every step of transformation in the state space of the proton subsystem should correspond to a definite step of rearrangement of the potential well for protons where they are dislocated.

One of the simplest forms of bistable potential is the polynomial

$$U(q) = \frac{1}{2}q^2(q^2 - 2),$$

and a necessary Hamiltonian has the form

$$H = \frac{1}{2}p^2 + \frac{1}{2}q^2(q^2 - 2).$$

So, if energy E is fixed, the time dependence $q(t)$ can be found from the elliptic integral

$$t - t_0 = \int_{q_0}^q \frac{dq_1}{\sqrt{2E + 2q_1^2 - q_1^4}}$$

and finally expressed in terms of the Jacobi function, but it is unnecessary to demonstrate this here.

The Hamiltonian of a direct sum of m such oscillators

$$H = \sum_{\mu=1}^m H_{\mu} = \frac{1}{2} \sum_{\mu=1}^m (p_{\mu}^2 - 2q_{\mu}^2 + q_{\mu}^4)$$

is to be subjected to an orthogonal pointwise transformation presented by the time dependent generating function

$$W(p, Q, t) = \sum_{\mu=1}^m \sum_{v=1}^m T_{\mu v}(t) p_{\mu} Q_v.$$

Its partial derivatives give expressions of old momenta p_{μ} and coordinates q_{μ} in terms of new ones P_{μ}, Q_{μ} :

$$\begin{aligned} P &= \frac{\partial}{\partial Q} W(p, Q, t), & q &= \frac{\partial}{\partial p} W(p, Q, t), \\ p_{\mu} &= \sum_v T_{\mu v}(t) p_v, & q_{\mu} &= \sum_v T_{\mu v}(t) Q_v. \end{aligned}$$

A new Hamiltonian which differs from the old one by the item $\frac{\partial}{\partial t} \Big|_{p=p(P)} W(p, Q, t)$ appears as

$$\tilde{H}(P, Q, t) = \frac{1}{2} \sum_{\mu} P_{\mu}^2 - \sum_{\mu} Q_{\mu}^2 + \frac{1}{2} \sum_{\mu} \left[\sum_v T_{\mu v}(t) Q_v \right]^4 + \sum_{\mu} \sum_v \dot{S}_{\mu v}(t) P_{\mu} Q_v,$$

where $S_{\mu\nu}(t)$ are elements of the skew-symmetric matrix $\hat{S}(t) = \ln \hat{T}(t)$ and $\dot{\hat{T}}(t) = \{T_{\mu\nu}(t)\}$, $\dot{S}_{\mu\nu}(t) = \frac{d}{dt}S_{\mu\nu}(t)$.

As soon as, in the ice I_h lattice, each proton has not more than 6 and not less than 1 protons neighboring with it, the sum over the index v in every term of the new Hamiltonian is to be calculated in the limits $1 \leq v \leq l$, $2 \leq l \leq 7$ (including a given proton) because another terms vanish. Number l depends on a phonon oscillations mode of the oxygen lattice.

Just above, the example of a vector fiber bundle model was demonstrated. Quite another way can be proposed on the base of a fiber bundle which has the nonabelian structure group $SU(2)$. If the well-known epimorphism $SU(2) \rightarrow SO(3)$ and trace metric $\langle \hat{H}_i, \hat{H}_j \rangle = \frac{1}{2}Tr \hat{H}_i \hat{H}_j$ are attracted, one can use the Pauli basis

$$\hat{h}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{h}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{h}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \langle \hat{h}_i, \hat{h}_j \rangle = \delta_{ij} \quad (i, j = \overline{1, 3})$$

in a linear space of traceless matrices $H_i \in L$. Then, vectors \mathbf{d}_i representing, for instance, a protons' i -dihedron dipole moment can be imaged as vector operators $\hat{\mathbf{d}}_i \in L$. Corresponding scalar product of \mathbf{d}_i over a hydrogen bond vector $\hat{\mathbf{n}}_{ij}$ may have a form

$$(\mathbf{d}_i, \mathbf{n}_{ij}) = \langle \chi_i | (\mathbf{d}_i \mathbf{n}_{ij}) | \chi_i \rangle$$

where χ_i are spinors.

The energy of dipole interaction between protons' dihedrons can be expressed as follows:

$$V = J_0 \sum_{(i,j) \in \Gamma} [\varepsilon(\mathbf{d}_i \mathbf{d}_j) - 3(\mathbf{d}_i \mathbf{n}_{ij})(\mathbf{d}_j \mathbf{n}_{ij})].$$

The sum must be accomplished by the whole interactions graph Γ . Here, J_0 is the energy constant and $\varepsilon < 1$ is a coefficient which allows taking into account the nondirect interaction between proton' dihedrons caused by oxygen electron shells. Going to the representation of a dihedron vector by corresponding spin matrices oriented along previously introduced basis vector \mathbf{e}_3 (lower) and \mathbf{e}'_3 (upper), one can obtain the formula

$$V = J_0 \sum_{(i,j) \in \Gamma} \langle \chi_i \chi_j | (\hat{H}_{ij}) | \chi_i \chi_j \rangle,$$

where bispinors $\chi_i \chi_j$ correspond to pairs of dihedrons situated at the endpoints of each hydrogen bond. In our case, Hamiltonians \hat{H}_{ij} are the next:

$$\hat{H}_{ij} = (\varepsilon - 3 \cos^2 \nu_{ij}) \hat{\sigma}_i^z \hat{\sigma}_j^z.$$

Fortunately, for the ice I_h structure, all the angles ν_{ij} between bonds' vectors \mathbf{n}_{ij} and \mathbf{e}_3 (or \mathbf{e}'_3) are identical and $\cos^2 \nu_{ij} = \frac{1}{3}$. So Hamiltonians have the very simple expression

$$\hat{H}_{ij} = (\varepsilon - 1) \hat{\sigma}_i^z \hat{\sigma}_j^z.$$

If indirect interaction was absent, all \hat{H}_{ij} were zero, but the presence of oxygen atoms makes ε much more less than unity ($0 < \varepsilon \ll 1$). Thus,

$$V = J \sum_{(i,j) \in \Gamma} \langle \chi_i \chi_j | \hat{\sigma}_i^z \hat{\sigma}_j^z | \chi_i \chi_j \rangle,$$

where $J = (\varepsilon - 1)J_0 < 0$. Finally, let us present the Hamiltonian in the explicit form

$$\begin{aligned} \hat{H} = J \sum_{(i,j) \in \Gamma} [& \hat{\sigma}_1^z(\mathbf{n}) \hat{\sigma}_2^z(\mathbf{n}) + \hat{\sigma}_2^z(\mathbf{n}) \hat{\sigma}_3^z(\mathbf{n}) + \hat{\sigma}_3^z(\mathbf{n}) \hat{\sigma}_4^z(\mathbf{n}) + \hat{\sigma}_1^z(\mathbf{n}) \hat{\sigma}_4^z(\mathbf{n} - \nu_3) + \\ & + \hat{\sigma}_1^z(\mathbf{n}) \hat{\sigma}_2^z(\mathbf{n} - \nu_1) + \hat{\sigma}_1^z(\mathbf{n} - \nu_2) \hat{\sigma}_2^z(\mathbf{n}) + \hat{\sigma}_3^z(\mathbf{n}) \hat{\sigma}_4^z(\mathbf{n} - \nu_2) + \hat{\sigma}_3^z(\mathbf{n} - \nu_1) \hat{\sigma}_4^z(\mathbf{n})] \end{aligned}$$

using notations

$$\mathbf{n} = \{n_1, n_2, n_3\}, \quad \nu_1 = \{1, 0, 0\}, \quad \nu_2 = \{0, 1, 0\}, \quad \nu_3 = \{0, 0, 1\},$$

$\hat{\sigma}_\alpha^z(\mathbf{n})$ is the spin operator of a dihedron $\mathbf{d}_\alpha(\mathbf{n})$ in the elementary cell with the number \mathbf{n} .

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