NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2020, 11 (1), P. 36–43

Geometrical analyses of nanostructures

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PACS 81.07.b, 81.07.D, 62.23.St, 61.50.Ah **DOI 10.17586/2220-8054-2020-11-1-36-43**

In this paper, the statistical and dynamical equivalence between rectangular cell and lower symmetry cell is presented. The achievement of this equivalence will improve theoretical investigations of nanostructures as thin film or quantum rods.

Keywords: Nanostructures, triclinic cell, cubic cell, thin film.

Received: 29 December 2019

1. Introduction

Nanotechnology has had much progress recently and produces different rectangular and cylindrical structures [1, 2]. The main problem of theoretical investigations of nanostructures is correct inclusion of boundary conditions into physical behavior of nanostructures. The importance of studying nanostructures is that their properties and behavior are different in comparison with the bulk structures.

The geometrical form of produced nanostructures is rectangular (thin films, quantum rods and quantum parallelepiped) or cylindrical (cylinders with nanocross-section and macroscopic height and cylinders having nanoheight and nanocross-section). Mentioned geometrical forms enable correct inclusion of boundary conditions into evaluations [3–10].

Taking into account of boundary conditions for the structure of lower symmetry (monoclinic, triclinic, tetragonal and others), we will try, in the first part of this paper, to achieve statistical equivalence between rectangular cell and lower symmetry cell. The statistical equivalence means equating of momentum volumes for the mentioned cells since statistical averages are usually calculated in momentum space.

In the second part, the rectangular cell will be reduced to simple cubic one which has the same momentum volume as lower symmetry one. After this, we can try to achieve the dynamical equivalence, too. In the nearest neighbors approximation, the dynamics of simple cubic cell is defined by six nearest neighbors. For lower symmetry cell the dynamics is defined by six or more neighbors. The last is dependent on angles between vectors of lower symmetry cell. If some of angles are less than 90°, then the interactions between ends of corresponding vectors have to be included into total interactions of atoms of lower symmetry cells. The achievement of described equivalence will noticeably accelerate theoretical investigations of nanostructures.

2. Preliminaries: Statistical equivalence

An elementary cell of triclinic crystal structure [11–13] has lattice constants: A, B and C. The lengths of these lattice constants are different and the angles between vectors $\vec{A}$, $\vec{B}$ and $\vec{C}$ are different: $\angle(\vec{A},\vec{B}) = \alpha$, $\angle(\vec{B},\vec{C}) = \beta$ and $\angle(\vec{C},\vec{A}) = \gamma$. The notations used are: $|\vec{A}| = A$, $|\vec{B}| = B$ and $|\vec{C}| = C$.

The lattice constant of rectangular structure will be denoted with a, b and c. Their lengths are different in general case. The angles between vectors $\vec{a}$, $\vec{b}$ and $\vec{c}$ are 90°. The notations used are $|\vec{a}| = a$, $|\vec{b}| = b$ and $|\vec{c}| = c$.

The elementary cells introduced are presented on Fig. 1 and Fig. 2.

The phase volume Φ is the product of configuration volume V and momentum volume W and, for crystals with simple lattice is equal to h^3 [14], where h is Planck's constant.

If configurationally, the volume of triclinic cell is denoted with V_T and the momentum cell volume with W_T, that results in the following:

$$V_T W_T = \Phi_T = h^3. \tag{1}$$

For rectangular structure we have the relation:

$$V_C W_C = \Phi_C = h^3, \tag{2}$$

where V_C is configurationally volume and W_C is momentum cell volume.

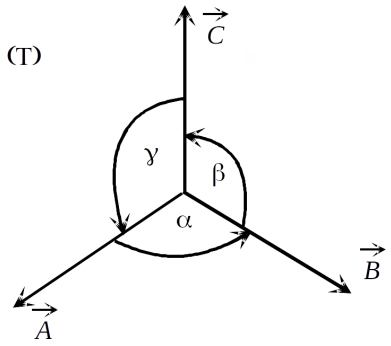

FIG. 1. Elementary cell of triclinic structure

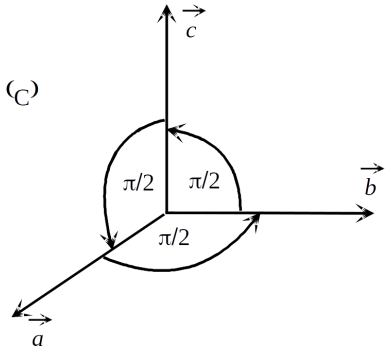

FIG. 2. Elementary cell of rectangular structure

In order to achieve equality:

$$V_C = V_T, \tag{3}$$

the rectangular vector $\vec{c}$ is chosen in the direction of vector $\vec{C}$ of triclinic cell and both of them, into direction of z-axis:

$$\vec{C} = C\vec{k}; \quad \vec{c} = c\vec{k}. \tag{4}$$

Vectors $\vec{a}$ and $\vec{b}$ of rectangular cell will be put in directions of x-axis and y-axis, respectively. In this way for rectangular structure can be written as:

$$\vec{a} = a\vec{i}; \quad \vec{b} = b\vec{j}; \quad \vec{c} = c\vec{k}, \tag{5}$$

where $\vec{i}$, $\vec{j}$ and $\vec{k}$ are vectors of Descartes coordinate system. Therefore, the expression for configurationally volume of rectangular structure is:

$$V_C = \vec{a}\left(\vec{b} \times \vec{c}\right) = \begin{vmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{vmatrix} = abc. \tag{6}$$

On the basis of (4), the configurational volume of the triclinic structure is given by:

$$V_T = \vec{A}\left(\vec{B} \times \vec{C}\right) = \begin{vmatrix} A_x & A_y & A_z \\ B_x & B_y & B_z \\ 0 & 0 & C \end{vmatrix} = C\left(A_x B_y - A_y B_x\right). \tag{7}$$

Using (6) and (7) the equality (3) becomes:

$$abc = \left(A_x B_y - A_y B_x\right) C. \tag{8}$$

From Fig. 3, in spherical coordinates, the projectors from (8) are:

$$\begin{aligned} A_x &= A\sin\gamma\cos\varphi_A; \quad B_x = B\sin\beta\cos\varphi_B; \\ A_y &= A\sin\gamma\sin\varphi_A; \quad B_y = B\sin\beta\sin\varphi_B; \\ A_z &= A\cos\gamma; \quad B_z = B\cos\beta \end{aligned} \tag{9}$$

and obtain:

$$A_x B_y - A_y B_x = AB\sin\beta\sin\gamma\sin\left(\varphi_B - \varphi_A\right). \tag{10}$$

Since

$$\vec{A} \circ \vec{B} = A_x B_x + A_y B_y + A_z B_z \tag{11}$$

the substitution of (9) leads to:

$$AB\cos\alpha = AB\sin\beta\sin\gamma\cos\left(\varphi_B - \varphi_A\right) + AB\cos\beta\cos\gamma. \tag{12}$$

Combining (12) and (10) results in the following:

$$\cos\left(\varphi_B - \varphi_A\right) = \frac{\cos\alpha - \cos\beta\cos\gamma}{\sin\beta\sin\gamma}. \tag{13}$$

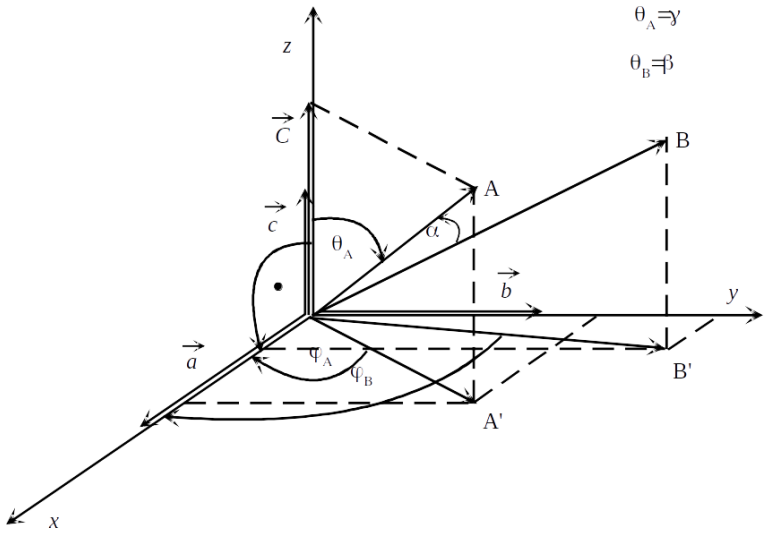

FIG. 3. Triclinic rectangular lattice vectors in spherical coordinates

Substituting (10) and (13) into (8), we finally obtain the connection between configurationally volumes of triclinic and rectangular cell:

$$abc = XABC, \tag{14}$$

where

$$X = \sqrt{1 + 2\cos\alpha\cos\beta\cos\gamma - \cos^2\alpha - \cos^2\beta - \cos^2\gamma}. \tag{15}$$

The formula (14) can be applied only if $X > 0$. In some cases the equivalence cannot be achieved. As an illustration if $\alpha = 90^\circ$, $\beta = 60^\circ$ and $\gamma = 30^\circ$, in accordance with (15), one obtains $X = 0$. For $\alpha = 150^\circ$, $\beta = 90^\circ$ and $\gamma = 30^\circ$ it follows from (15) that $X = -0.5$. In both cases the equivalence cannot be achieved. The cases when the exposed procedure gives satisfactory result are for example $\alpha = \beta = \gamma = 1^\circ$ with $X = 6.9 \cdot 10^{-8}$, $\alpha = 70^\circ$, $\beta = 50^\circ$ and $\gamma = 30^\circ$ with $X = 0.312$, $\alpha = 110^\circ$, $\beta = 100^\circ$ and $\gamma = 80^\circ$ with $X = 0.843$ etc. For $\alpha = 125.9^\circ$, $\beta = 115.3^\circ$ and $\gamma = 115.1^\circ$ results $X = 0.081$, i.e. this has equivalent cubic cell.

It should be pointed out that transition to statistically equivalent cell is possible for all monoclinic structures [15]. In these structures, two angles are equal 90° and in accordance with (14) it follows $X = 1 - \cos^2\beta$, where $\beta \neq 90^\circ$, i.e. we always have that $X > 0$.

It is clear, also, that the equivalence conditions are not uniquely defined.

Momentum cell volume is defined as product of reciprocal configurationally cell and factor $(h/2\pi)^3$. The vectors $\vec{k}_a$, $\vec{k}_b$ and $\vec{k}_c$ are defined as follows:

$$\vec{k}_a = 2\pi\frac{\vec{a}\times\vec{c}}{\vec{a}\cdot\left(\vec{b}\times\vec{c}\right)} = \frac{2\pi}{a}\vec{i}; \quad \vec{k}_b = 2\pi\frac{\vec{c}\times\vec{a}}{\vec{b}\cdot(\vec{c}\times\vec{a})} = \frac{2\pi}{b}\vec{j}; \quad \vec{k}_c = 2\pi\frac{\vec{a}\times\vec{b}}{\vec{c}\cdot\left(\vec{a}\times\vec{b}\right)} = \frac{2\pi}{c}\vec{k}. \tag{16}$$

Taking into account formula (6) we easily conclude on the basis of (16) that the volume of reciprocal cell is:

$$R = \frac{(2\pi)^3}{abc}. \tag{17}$$

Multiplying (17) with we obtain volume of momentum cell for rectangular structure:

$$W_C = \frac{h^3}{abc} = W_T. \tag{18}$$

The last equality sign follows from the fact that equality of configurationally cells V_C and V_T has been achieved.

If one considers:

$$a = X^p A; \quad b = X^q B; \quad c = X^r C, \tag{19}$$

where p, q and k are arbitrary constants, (14) gives

$$p + q + r = \frac{1}{2}. \tag{20}$$

In order to obtain equivalent simple cubic cell, one takes

$$\frac{a}{b} = X^{p-q}\frac{A}{B} = 1. \tag{21}$$

$$\frac{a}{c} = X^{p-r}\frac{A}{C} = 1. \tag{22}$$

Combining (20), (21) and (22) we find

$$p = \frac{1}{6} - \frac{2\ln A - \ln B - \ln C}{3\ln X}. \tag{23}$$

Taking $\frac{b}{a} = X^{q-p}\frac{B}{A}$, $\frac{b}{c} = X^{q-r}\frac{B}{C}$, we have:

$$q = \frac{1}{6} - \frac{2\ln B - \ln A - \ln C}{3\ln X}. \tag{24}$$

Finally taking $\frac{c}{a} = X^{r-p}\frac{C}{A}$, $\frac{c}{b} = X^{r-q}\frac{C}{B}$, we get:

$$r = \frac{1}{6} - \frac{2\ln C - \ln A - \ln B}{3\ln X}. \tag{25}$$

Substituting (23), (24) and (25) into (14) it obtain the constant of simple cubic lattice which is statistically equivalent to triclinic one with lattice constants A, B and C.

$$d = X^p A = X^q B = X^r C. \tag{26}$$

For the angles $\alpha = 125.9^\circ$, $\beta = 115.3^\circ$ and $\gamma = 115.1^\circ$, while the lattice constants are $A = 0.942$, $B = 1.264$ and $C = 0.573$ nm the value of d, is calculated by means of (23), (24) and (25) is $d = 0.839$ nm.

3. Results: Dynamical equivalence of triclinic cell and simple cubic cell

The achievement of this equivalence requires knowing of interactions between atoms (molecules) of triclinic cell. Using Landau's estimate [16] of intermolecular interactions, i.e. we assume that interaction between two atoms is of the form:

$$I(l) = \begin{cases} \frac{\varphi}{l^\eta}; & l > 1\,\text{nm}; \\ \frac{\varphi}{l^{-\eta}}; & l < 1\,\text{nm}; \end{cases} \qquad \eta > 0, \tag{27}$$

where φ is interaction constant expressed in $J \times \left(10^{-9}\,\text{m}\right)^{\pm\eta}$, while l is distance between nearest neighbors expressed in 10^{-9} m.

The total interaction energy of triclinic cell is given as:

$$J_T = 2\varphi\left(\frac{1}{A^{-\eta}} + \frac{1}{B^{-\eta}} + \frac{1}{C^{-\eta}} + \frac{1}{(AB)^{-\eta}} + \frac{1}{(AC)^{-\eta}} + \frac{1}{(BC)^{-\eta}}\right), \tag{28}$$

since all lengths are less than 1 nm. The formula is valid if $A \geq B$, C, AB, AC, BC. If some of lengths AB, AC and BC is higher than A, this term has to be omitted from (28).

The total interaction energy of the equivalent simple cubic cell is given by:

$$J_{SC} = \frac{6\Phi}{d^{-\eta}}, \quad d < 1\,\text{nm}, \tag{29}$$

where Φ is interaction constant of equivalent simple cubic cell.

It is obvious that the structures will be dynamically equivalent if

$$\Phi = \frac{\varphi}{3}d^\eta\left(\frac{1}{A^{-\eta}} + \frac{1}{B^{-\eta}} + \frac{1}{C^{-\eta}} + \frac{1}{(AB)^{-\eta}} + \frac{1}{(AC)^{-\eta}} + \frac{1}{(BC)^{-\eta}}\right). \tag{30}$$

For calculation of some physical characteristics of simple cubic lattice, the interaction between two neighbors is most often used. This interaction is $j_{CE} = \frac{\Phi}{d^{-\eta}}$, i.e. in accordance with (30):

$$j_{CE} = \frac{\varphi}{3}\left(\frac{1}{A^{-\eta}} + \frac{1}{B^{-\eta}} + \frac{1}{C^{-\eta}} + \frac{1}{(AB)^{-\eta}} + \frac{1}{(AC)^{-\eta}} + \frac{1}{(BC)^{-\eta}}\right). \tag{31}$$

An illustrative example is the ideal Heisenberg ferromagnet with spin $S = 1/2$ in Bloch's approximation. The exchange interactions are, in accordance with general opinion, of exponential type [14]. It means that in formula (31) every of terms have to be prescribed in following way

$$\frac{1}{L^{-\eta}} = e^{\ln \frac{1}{L^{-eta}}} = e^{\eta \ln L} \quad (l < 1).$$

The Hamiltonian of this system in nearest neighbour's approximation [8] is:

$$H = 3j_{CE} \sum_{n_x,n_y,n_z} B^+_{n_x,n_y,n_z} B_{n_x,n_y,n_z} - \frac{1}{2} j_{CE} \sum_{n_x,n_y,n_z} B^+_{n_x,n_y,n_z} \Big(B_{n_x+1,n_y,n_z} + B_{n_x-1,n_y,n_z} + B_{n_x,n_y+1,n_z} + B_{n_x,n_y-1,n_z} + B_{n_x,n_y,n_z+1} + B_{n_x,n_y,n_z-1} \Big) \quad (32)$$

with B_{n_x,n_y,n_z} Bose operators.

The dispersion law of spin waves is:

$$E_{k_x,k_y,k_z} = (3 - \cos k_x d - \cos k_y d - \cos k_z d)\, j_{CE} \approx \frac{1}{2} j_{CE} k^2 d^2. \quad (33)$$

The ordering parameter in Bloch's approximation is given by:

$$\sigma = 1 - 2\langle B^+ B \rangle = 1 - 2\zeta_{3/2} \tau^{3/2}, \quad (34)$$

where

$$\zeta_{3/2} = \sum_{n=1}^{\infty} \frac{1}{n^{3/2}} \quad (35)$$

is Riemann's function [14], while:

$$\tau = \frac{k_B T}{2\pi} \frac{1}{j_{CE}}. \quad (36)$$

As it is seen, the value j_{CE} is expressed in parameters of triclinic structure (see formula (31) and, consequently, the result (34) with τ expressed by (36) represents ordering parameter of ferromagnet with triclinic lattice which is evaluated by means of equivalent simple cubic lattice.

The given example demonstrates the advantages of translation the lower symmetry structure into equivalent simple cubic one. The statistical averages can be evaluated without mathematical complication and by means of standard and well developed approaches.

The more complicated problem is determining of ordering parameter of thin film cut off from triclinic crystal. In this case we immediately go over to thin film of statistically and dynamically equivalent simple cubic structure. The interactions j_{CE} are given by (31).

The Hamiltonian of equivalent film in nearest neighbor's approximation [5] is given by:

$$H = \frac{1}{2} \sum_{n_x,n_y,n_z} \Big(j_{n_x+1,n_y,n_z;n_x,n_y,n_z} + j_{n_x-1,n_y,n_z;n_x,n_y,n_z} + j_{n_x,n_y+1,n_z;n_x,n_y,n_z} + j_{n_x,n_y-1,n_z;n_x,n_y,n_z} + j_{n_z,n_y,n_z+1;n_x,n_y,n_z} + j_{n_x,n_y,n_z-1;n_x,n_y,n_z} \Big) B^+_{n_x,n_y,n_z} B_{n_x,n_y,n_z} - j_{n_x,n_y,n_z-1;n_x,n_y,n_z} B^+_{n_x,n_y,n_z} B_{n_x,n_y,n_z} - \frac{1}{2} \sum_{n_x,n_y,n_z} B^+_{n_x,n_y,n_z} \Big(j_{n_x+1,n_y,n_z;n_x,n_y,n_z} B^+_{n_x+1,n_y,n_z} + j_{n_x-1,n_y,n_z;n_x,n_y,n_z} B^+_{n_x-1,n_y,n_z} + j_{n_x,n_y+1,n_z;n_x,n_y,n_z} B^+_{n_x,n_y+1,n_z} + j_{n_x,n_y,n_z+1;n_x,n_y,n_z} B^+_{n_x,n_y,n_z+1} + j_{n_x,n_y,n_z-1;n_x,n_y,n_z} B^+_{n_x,n_y,n_z-1} \Big). \quad (37)$$

For functions j the following is valid:

$$j_{n_x \pm 1,n_y,n_z;n_x,n_y,n_z} = j_{n_x,n_y \pm,n_z+1;n_x,n_y,n_z} = j_{n_x,n_y,n_z \pm 1;n_x,n_y,n_z} = j_{CE}. \quad (38)$$

The cut off in z direction leads to the following boundary conditions:

$$j_{n_x,n_y,-1;n_x,n_y,0} = j_{n_x,n_y,N_z+1;n_x,n_y,N_z} = 0. \quad (39)$$

The film will be analysed by means of Green's function:

$$G_{n_x,n_y,n_z;m_x,m_y,m_z}(t) = \Big\langle \Big\langle B_{n_x,n_y,n_z}(t) \Big| B^+_{n_x,n_y,n_z}(0) \Big\rangle \Big\rangle = \Theta(t) \Big\langle \Big[B_{n_x,n_y,n_z}(t), B^+_{n_x,n_y,n_z}(0) \Big] \Big\rangle; \quad (40)$$

where $\Theta(t) = \begin{cases} 1, & t > 0; \\ 0, & t < 0; \end{cases}$ is the Heaviside step function.

Fourier transformations are:

$$G_{n_x,n_y,n_z;m_x,m_y,m_z}(t) = \int\limits_{-\infty}^{+\infty} d\omega \mathrm{e}^{-i\omega t} G_{n_x,n_y,n_z;m_x,m_y,m_z}(\omega); \quad \delta(t) = \frac{1}{2\pi} \int\limits_{-\infty}^{+\infty} d\omega \mathrm{e}^{-i\omega t}. \tag{41}$$

In order to use translational invariance in x, y planes the following transformation is used [17, 18]

$$G_{n_x,n_y,n_z;m_x,m_y,m_z}(\omega) = \frac{1}{N_x N_y} \sum_{k_x,k_y} \mathrm{e}^{idk_x(n_x-m_x)+idk_y(n_y-m_y)} \Gamma(k_x, k_y, \omega). \tag{42}$$

The quoted procedure gives the system of three different equations:

$$\frac{1}{2} j_{CE} \left(\Gamma_{n_z+1,m_z} + \Gamma_{n_z-1,m_z}\right) + \rho \Gamma_{n_z,m_z} = \frac{i\hbar}{2\pi} \delta_{n_z,m_z}; \quad 1 \le n_z \le N_z - 1, \tag{43}$$

$$\frac{1}{2} j_{CE} \Gamma_{1,m_z} + \left(\rho + \frac{1}{2} j_{CE}\right) \Gamma_{0,m_z} = \frac{i\hbar}{2\pi} \delta_{0,m_z}, \tag{44}$$

$$\frac{1}{2} j_{CE} \Gamma_{N_z-1,m_z} + \left(\rho + \frac{1}{2} j_{CE}\right) \Gamma_{N_z,m_z} = \frac{i\hbar}{2\pi} \delta_{N_z,m_z}; \quad n_z = N_z, \tag{45}$$

where

$$\rho = E - 3 j_{CE} + j_{CE} (\cos dk_x + \cos dk_y). \tag{46}$$

It can be easily shown that by the substitution:

$$\Gamma_{n_z;m_z}(\omega) = \sum_{\lambda=1}^{N_z} g(k_x, k_y, \lambda; \omega)\, \Omega_\lambda(m_z) F_\lambda(n_z), \tag{47}$$

where Ω are undetermined functions and F is given by:

$$F_\lambda(n_z) = \sin(n_z + 1) \frac{\pi\lambda}{N_z + 1} - \sin n_z \frac{\pi\lambda}{N_z + 1}; \quad \lambda = 1, 2, 3, ..., N_z, \tag{48}$$

the system of equations (43), (44) and (45) reduces into one equation of the form

$$\sum_{\lambda=1}^{N_z} g(k_x, k_y, \lambda; \omega) \left(j_{CE} \cos\frac{\pi\lambda}{N_z + 1} + \rho\right) \Omega_\lambda(m_z) F_\lambda(n_z) = \frac{i\hbar}{2\pi} \delta_{n_z,m_z}; \quad n_z = 0, 1, 2, ..., N_z. \tag{49}$$

Kronecker symbol will be taken in the form

$$\delta_{n_z,m_z} = \sum_{\lambda=1}^{N_z} \Omega_\lambda(m_z) F_\lambda(n_z). \tag{50}$$

Using the properties of Kronecker symbol $\delta_{n_z,n_z} = 1$ and $\delta_{n_z,m_z} = 0$, $n_z \neq m_z$, we obtain the system of n_z^2 algebraic equations determining unknown functions Ω.

$$g(k_x, k_y, \lambda; \omega) = \frac{i\hbar}{2\pi} \frac{1}{j_{CE} \cos\frac{\pi\lambda}{N_z+1} + \rho} = \frac{i\hbar}{2\pi} \frac{1}{E - E_{k_x,k_y}}, \tag{51}$$

where

$$E_{k_x,k_y,\lambda} = 3 j_{CE} - j_{CE} \left(\cos k_x d + \cos k_y d + \cos\frac{\pi\lambda}{N_z + 1}\right). \tag{52}$$

Substituting (51) into (47) and including obtained result into (42) we get final result for Green's function:

$$G_{n_x,n_y,n_z;m_x,m_y,m_z}(\omega) = \frac{i}{2\pi} \frac{1}{N_x N_y} \sum_{k_x,k_y} \mathrm{e}^{idk_x(n_x-m_x)+idk_y(n_y-m_y)} \sum_{\lambda=1}^{N_z} \frac{\Omega_\lambda(m_z) F_\lambda(n_z)}{\omega - \omega_{k_x,k_y,\lambda}}, \tag{53}$$

where

$$\omega = \frac{E}{\hbar}, \quad \omega_{k_x,k_y,\lambda} = \frac{E_{k_x,k_y,\lambda}}{\hbar}. \tag{54}$$

The expression for concentration is:

$$\left\langle B^+_{n_x,n_y,n_z}(0)\, B_{n_x,n_y,n_z}(t) \right\rangle = \frac{1}{N_x N_y} \sum_{k_x,k_y} \sum_{\lambda=1}^{N_z} \frac{\Omega_\lambda(m_z) F_\lambda(n_z)}{\omega - \omega_{k_x,k_y,\lambda}}. \tag{55}$$

It is very important to note that the transformation from configurational space to momentum space is not isomorphic one. It is transition of the type $n \to n-1$ [8]. It is seen that for N_z+1 values of index n_z the momentum index λ takes N_z values. It practically means that in one of layers of the film there are not spin waves. In further we shall consider three layer films. Due to the mentioned reduction it goes over to three subfilms containing two layers.

For subfilm 0–1 from Fig. 4, the solutions of the equation:

$$\delta_{m_z,n_z} = \sum_{\lambda=1}^{2} \Omega_\lambda\left(m_z\right) F_\lambda\left(m_z\right); \quad n_z, m_z \in (0,1)\,, \tag{56}$$

are

$$\Omega_1\left(0\right) = 2\frac{\sqrt{3}}{3}; \quad \Omega_2\left(0\right) = 0; \quad \Omega_1\left(1\right) = \frac{\sqrt{3}}{3}; \quad \Omega_2\left(1\right) = -\frac{\sqrt{3}}{3}. \tag{57}$$

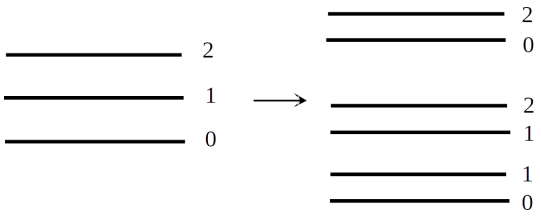

FIG. 4. The Autoreduction in three layer film

Substituting (57) into (55) it obtain concentrations:

$$\langle B^+B\rangle_{n_z=0} = \frac{1}{4\sqrt{\pi}}\frac{\theta}{j_{CE}}\sum_{n=1}^{\infty}\frac{1}{n}e^{-\frac{j_{CE}}{2\theta}n}; \quad \langle B^+B\rangle_{n_z=1} = \frac{1}{4\sqrt{\pi}}\frac{\theta}{j_{CE}}\sum_{n=1}^{\infty}\frac{1}{n}e^{-\frac{3j_{CE}}{2\theta}n}, \tag{58}$$

where $\theta = k_BT$.

It is seen that concentration of the layers 0 and 1 differ. It is the consequence of broken symmetry. The corresponding ordering parameters are:

$$\sigma_{n_z=0} = 1 - \frac{1}{2\sqrt{\pi}}\frac{\theta}{j_{CE}}\sum_{n=1}^{\infty}\frac{1}{n}e^{-\frac{j_{CE}}{2\theta}n}; \quad \sigma_{n_z=1} = 1 - \frac{1}{2\sqrt{\pi}}\frac{\theta}{j_{CE}}\sum_{n=1}^{\infty}\frac{1}{n}e^{-\frac{3j_{CE}}{2\theta}n}. \tag{59}$$

The last result shows that the layer $n_z = 1$ is better ordered. It is physically understandable since to spin in layer $n_z = 1$ act exchange forces from two sides, while to spins of layer $n_z = 0$ act exchange forces from one side, only. In the same way for subfilm 1–2 we have:

$$\langle B^+B\rangle_{n_z=2} = \frac{1}{4\sqrt{\pi}}\frac{\theta}{j_{CE}}\sum_{n=1}^{\infty}\frac{1}{n}e^{-\frac{j_{CE}}{2\theta}n}; \quad \langle B^+B\rangle_{n_z=1} = \frac{1}{4\sqrt{\pi}}\frac{\theta}{j_{CE}}\sum_{n=1}^{\infty}\frac{1}{n}e^{-\frac{3j_{CE}}{2\theta}n}, \tag{60}$$

$$\sigma_{n_z=2} = 1 - \frac{1}{2\sqrt{\pi}}\frac{\theta}{j_{CE}}\sum_{n=1}^{\infty}\frac{1}{n}e^{-\frac{j_{CE}}{2\theta}n}; \quad \sigma_{n_z=1} = 1 - \frac{1}{2\sqrt{\pi}}\frac{\theta}{j_{CE}}\sum_{n=1}^{\infty}\frac{1}{n}e^{-\frac{3j_{CE}}{2\theta}n}. \tag{61}$$

Finally for subfilm 0–2 we have:

$$\langle B^+B\rangle_{n_z=0} = \langle B^+B\rangle_{n_z=2} = \frac{1}{8\sqrt{\pi}}\frac{\theta}{j_{CE}}\left(\sum_{n=1}^{\infty}\frac{1}{n}e^{-\frac{j_{CE}}{2\theta}n} + \sum_{n=1}^{\infty}\frac{1}{n}e^{-\frac{3j_{CE}}{2\theta}n}\right); \tag{62}$$

$$\sigma_{n_z=0} = \sigma_{n_z=2} = 1 - \frac{1}{4\sqrt{\pi}}\frac{\theta}{j_{CE}}\left(\sum_{n=1}^{\infty}\frac{1}{n}e^{-\frac{j_{CE}}{2\theta}n} + \sum_{n=1}^{\infty}\frac{1}{n}e^{-\frac{3j_{CE}}{2\theta}n}\right). \tag{63}$$

The obtained results are in full accordance with symmetry of structure.

4. Conclusions

The recovery of equivalence between rectangular structures and the structures of lower symmetry (triclinic, monoclinic, etc.) is one of the most important necessities the theory of nanostructures. The theoretical analysis of nanostructures is developed for rectangular and cylindrical ones. In this work, the concept of statistical and dynamical equivalence between structures of higher and lower symmetry was introduced.

The proposed method is not universal, unfortunately. As it was seen for some triclinic structures the equivalent rectangular one does not exist. Nevertheless, in many actual cases method of equivalence can be applied. Concerning the monoclinic structure this method is always successful.

Acknowledgements

This work was supported by a grant of the Romanian Ministry of Research and Innovation, project number 10PFE/16.10.2018, PERFORM-TECH-UPT – The increasing of the institutional performance of the Polytechnic University of Timişoara by strengthening the research, development and technological transfer capacity in the field of "Energy, Environment and Climate Change", within Program 1 – Development of the national system of Research and Development, Subprogram 1.2 – Institutional Performance – Institutional Development Projects – Excellence Funding Projects in RDI, PNCDI III.

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