Green's Function Method Approach to Electron Configuration of Superlattices

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Abstract

As quantum low-dimensional structures are of current interest, we tried to study the basic microscopic behaviour of electron subsystem in superlattices. The microtheoretical method of two-time temperature dependent Green's functions was applied for the calculation of electron energy spectra and spectral weights of electrons in superlattices (crystalline structures formed by alternating thin films with changed energy transfer between them). These analysis were performed combining the analytical (using the matrix representation of Chebishev's polynomials) and numerical (using the programme *Mathematica*) approach leading to interesting results for the explanation of some physical properties of these structures.

Key words and phrases: superlattices, electron configuration, Green's functions.

1 Introduction

During the last few decades superlattices have been the subject of intensive experimental and theoretical studies because of potential applications in electronic devices and the large variety of transport and physical phenomena of these materials [1,2]. Consequently, many efforts have been made to determine the electronic structure of these materials using the different methods of calculation [3-6].

Typical example of superlattices are multi-layered crystalline structures type $(AC)_m(BC)_n$, formed by alternating super-layers of m layers of the first two-component compound AC and n layers of the second compound BC, along the direction of crystal growth [4]. On the basic our previous paper, related to crystalline thin film model [7,8], we perform Green's function method in order to calculate electron dispersion law and spectral weights of electrons in superlattice. Influence of electron energy transfer between and inside super-layers to electron spectra and states was analyzed.

2 Dispersion law of electrons

Figure 1 represents model of superlattice, which is formed by alternating super-layers (thin films) of n_a (thickness d_1) layers of constituent A and n_b layers (thickness d_2) of constituent B (model of periodically superlattice [3,4,6]) along z direction, while it is infinite along x and y directions. Crystal parameters along x and y directions must the be same ($a_x^a = a_x^b = a_x$ and $a_y^a = a_y^b = a_y$), because the structure must not be stressed; while parameters along z direction may be different ($a_z^a = a^a \neq a_z^b = a^b$ and $a_z^{a-b} = a$).

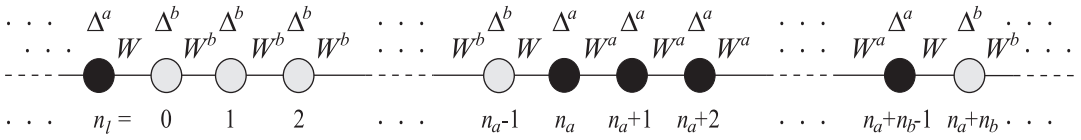

Figure 1: Position of electrons along z-direction in superlattice

We base our analysis of electronic subsystem on the standard tight-binding electron Hamiltonian (of modeled structure) in harmonic and nearest-neighbor approximation [5-8]:

$$
\begin{aligned}
H = & \sum_{m_{x/y/z}=-N_{x/y/z}/2}^{N_{x/y/z}/2} \left\{ \sum_{m_l=0}^{n_a-1} \Delta^a a^+_{m_x m_y m_z m_l} a_{m_x m_y m_z m_l} + \right. \\
+ & \sum_{m_l=n_a}^{n_a+n_b-1} \Delta^b a^+_{m_x m_y m_z m_l} a_{m_x m_y m_z m_l} - \\
- & \sum_{m_l=1}^{n_a-2} W^a a^+_{m_x m_y m_z m_l} \left(a_{m_x m_y m_z m_l-1} + a_{m_x m_y m_z m_l+1} \right) - \\
- & \sum_{m_l=n_a+1}^{n_a+n_b-2} W^b a^+_{m_x m_y m_z m_l} \left(a_{m_x m_y m_z m_l-1} + a_{m_x m_y m_z m_l+1} \right) - \\
- & a^+_{m_x m_y m_z,0} \left(W a_{m_x m_y m_z-1,n_a+n_b-1} + W^a a_{m_x m_y m_z,1} \right) - \\
- & a^+_{m_x m_y m_z,n_a-1} \left(W^a a_{m_x m_y m_z,n_a-2} + W a_{m_x m_y m_z,n_a} \right) - \\
- & a^+_{m_x m_y m_z,n_a} \left(W a_{m_x m_y m_z,n_a-1} + W^b a_{m_x m_y m_z,n_a+1} \right) - \\
- & a^+_{m_x m_y m_z,n_a+n_b-1} \left(W^b a_{m_x m_y m_z,n_a+n_b-2} + W a_{m_x m_y m_z+1,0} \right) - \\
- & \sum_{m_l} \left[W_x^{a/b} a^+_{m_x m_y m_z m_l} \left(a_{m_x-1,m_y m_z m_l} + a_{m_x+1,m_y m_z m_l} \right) + \right. \\
+ & \left. \left. W_y^{a/b} a^+_{m_x m_y m_z m_l} \left(a_{m_x m_y-1,m_z m_l} + a_{m_x m_y+1,m_z m_l} \right) \right] \right\} ,
\end{aligned}
\tag{1}
$$

where $\Delta^{a/b}$ denotes the energy of electron localization on crystal sites, while $W_x^{a/b}$, $W_y^{a/b}$ and $W^{a/b}$ represent energy transfer between electrons inside super-layers along x, y and z directions, respectively; W is electron energy transfer between super-layers along z direction; $m_{x/y}$ are site index along x or y direction; m_z is super-layer index (along z direction), while $m_l \in [0, n_a + n_b - 1]$ is site index inside super-layer. Using the cycling conditions for x and y

coordinates: $f_{m_x m_y m_z m_l + N_{x/y}} = f_{m_x m_y m_z m_l} \;\Rightarrow\; \mathrm{e}^{iN_{x/y}k_{x/y}a_{x/y}} = \mathrm{e}^{2\pi\nu_{x/y}i}$, we can write cycling condition for super-layer along z-direction:

$$f_{m_x m_y m_z m_l + (n_a+n_b)N_z} = f_{m_x m_y m_z m_l} \;;\Rightarrow\; \mathrm{e}^{i(n_a+n_b)N_z k_z \tilde{a}} = \mathrm{e}^{2\pi\nu_z i} \; . \tag{2}$$

Allowed values of k_z can be counted by counter $\nu_z \in 0, \pm 1, \pm 2, ..., \pm N_z/2$. On that way, we can define the limits of the first Brillouin zone (BZ) along z direction [9,10]:

$$k_z \in \left[-\frac{\pi}{(n_a+n_b)\tilde{a}}, +\frac{\pi}{(n_a+n_b)\tilde{a}} \right] \;; \quad \tilde{a} = \frac{(n_a-1)a^a + (n_b-1)a^b + 2a}{n_a+n_b} \; , \tag{3}$$

where $\tilde{a}$ is mean value of interlayer distance along z direction.

In order to find electron dispersion law of superlattice we shall calculate single-particle anti-commutator Green's function, using the Hamiltonian (1):

$$G_{\vec{n}n_l;\vec{m}m_l} = \Theta(t)\langle\left\{ a_{n_x n_y n_z n_l}, a^+_{m_x m_y m_z m_l} \right\}\rangle \; . \tag{4}$$

After time Fourier transform we get equation of motion for Green's function:

$$\begin{aligned} & \hbar\omega G_{\vec{n};\vec{m}} = \frac{i\hbar}{2\pi}\delta_{\vec{n};\vec{m}} + \Delta_{\vec{n}} G_{\vec{n};\vec{m}} - \\ - \;& W^{\vec{n}}_x \left(G_{n_x-1,n_y n_z n_l;\vec{m}} + G_{n_x+1,n_y n_z n_l;\vec{m}} \right) - W^{\vec{n}}_y \left(G_{n_x n_y-1,n_z n_l;\vec{m}} + G_{n_x n_y+1,n_z n_l;\vec{m}} \right) - \\ - \;& W_{\vec{n};n_x n_y n_z n_l-1} G_{n_x n_y n_z n_l-1;\vec{m}} - W_{\vec{n};n_x n_y n_z n_l+1} G_{n_x n_y n_z n_l+1;\vec{m}} \; , \end{aligned} \tag{5}$$

where $\Delta \in \{\Delta_a, \Delta_b\}$, $W^{\vec{n}}_{x/y} \in \{W^a_{x/y}, W^b_{x/y}\}$ and $W_{\vec{n};n_x n_y n_z n_l \pm 1} \in \{W^a, W^b, W\}$, depending on position in super-layer.

Performing partial spatial (xyz) Fourier transform (because translational symmetry is broken for index l):

$$f_{\vec{n};\vec{m}} = \frac{1}{N_x N_y N_z} \sum_{k_x k_y k_z} f_{n_l;m_l} \, \mathrm{e}^{i[a_x k_x (n_x - m_x) + a_y k_y (n_y - m_y) + \tilde{a}(n_a+n_b)k_z (n_z - m_z) + J]} \; , \tag{6}$$

$$J = \begin{cases} 1.\; a^a k_z (n_l - m_l) & , \;\; n_l - m_l < n_a \\ 2.\; a^a k_z (n_a - 1) + a k_z & , \;\; n_l - m_l = n_a \\ 3.\; a^a k_z (n_a - 1) + a k_z + a^b k_z (n_l - m_l - n_a) & , \;\; n_a < n_l - m_l < n_a + n_b \\ 4.\; a^a k_z (n_a - 1) + a^b k_z (n_b - 1) + 2 a k_z & , \;\; n_l - m_l = n_a + n_b \end{cases} \tag{7}$$

we obtain the system of $n_a + n_b$ nonhomogenious algebraic-difference equations for Green's functions [6,9,10]:

$$\begin{aligned} [\hbar\omega \;& - \; \Delta^a + 2\left(W^a_x \cos a_x k_x + W^a_y \cos a_y k_y \right) \Big] G_0 + \\ & + \; W G_{n_a+n_b-1} \mathrm{e}^{-ia k_z} + W^a G_1 \mathrm{e}^{ia^a k_z} = \frac{i\hbar}{2\pi}\delta_0 \\ [\hbar\omega \;& - \; \Delta^a + 2\left(W^a_x \cos a_x k_x + W^a_y \cos a_y k_y \right) \Big] G_1 + \\ & + \; W^a \left(G_0 \mathrm{e}^{-ia^a k_z} + G_2 \mathrm{e}^{ia^a k_z} \right) = \frac{i\hbar}{2\pi}\delta_1 \end{aligned}$$

$$* \qquad * \qquad * \qquad *$$

$$
\begin{aligned}
[\hbar\omega &- \Delta^a + 2\left(W_x^a \cos a_x k_x + W_y^a \cos a_y k_y\right)] G_{n_a-2} + \\
&+ W^a \left(G_{n_a-3} \mathrm{e}^{-ia^a k_z} + G_{n_a-1} \mathrm{e}^{ia^a k_z}\right) = \frac{i\hbar}{2\pi} \delta_{n_a-2} \\
[\hbar\omega &- \Delta^a + 2\left(W_x^a \cos a_x k_x + W_y^a \cos a_y k_y\right)] G_{n_a-1} + \\
&+ W^a G_{n_a-2} \mathrm{e}^{-ia^a k_z} + W G_{n_a} \mathrm{e}^{iak_z} = \frac{i\hbar}{2\pi} \delta_{n_a-1} \\
[\hbar\omega &- \Delta^b + 2\left(W_x^b \cos a_x k_x + W_y^b \cos a_y k_y\right)] G_{n_a} + \\
&+ W G_{n_a-1} \mathrm{e}^{-iak_z} + W^b G_{n_a+1} \mathrm{e}^{ia^b k_z} = \frac{i\hbar}{2\pi} \delta_{n_a} \\
[\hbar\omega &- \Delta^b + 2\left(W_x^b \cos a_x k_x + W_y^b \cos a_y k_y\right)] G_{n_a+1} + \\
&+ W^b \left(G_{n_a} \mathrm{e}^{-ia^b k_z} + G_{n_a+2} \mathrm{e}^{ia^b k_z}\right) = \frac{i\hbar}{2\pi} \delta_{n_a+1} \\
& \quad * \qquad * \qquad * \qquad * \\
[\hbar\omega &- \Delta^b + 2\left(W_x^b \cos a_x k_x + W_y^b \cos a_y k_y\right)] G_{n_a+n_b-2} + \\
&+ W^b \left(G_{n_a+n_b-3} \mathrm{e}^{-ia^b k_z} + G_{n_a+n_b-1} \mathrm{e}^{ia^b k_z}\right) = \frac{i\hbar}{2\pi} \delta_{n_a+n_b-2} \\
[\hbar\omega &- \Delta^b + 2\left(W_x^b \cos a_x k_x + W_y^b \cos a_y k_y\right)] G_{n_a+n_b-1} + \\
&+ W^b G_{n_a+n_b-2} \mathrm{e}^{-ia^b k_z} + W + G_0 \mathrm{e}^{iak_z} = \frac{i\hbar}{2\pi} \delta_{n_a+n_b-1} \, .
\end{aligned}
\tag{8}
$$

There are only $n_a + n_b$ different Green's functions, because super-layers formed of $n_a + n_b$ nonequivalent crystal layers (count by index l). Therefore, we wrote above system using relation: $G_{n_x n_y n_z n_l + (n_a+n_b)} = G_{n_x n_y n_z n_l}$.

We simplified model studying simple cubic lattice, where: $a^a = a^b = \tilde{a} = a = a_z$ and $a_x^{a/b} = a_y^{a/b} = a_z = a$. Introducing the following shortnotes: $W_{x/y}^a/W = W^a/W = \alpha$, $W_{x/y}^b/W = W^b/W = \beta$, $F = 2\left(\cos ak_x + \cos ak_y\right)$ we can write determinant of system in form:

$$
\left[\begin{array}{ccc|cccc|ccc}
\varrho_\alpha & \alpha\, \mathrm{e}^{iak_z} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathrm{e}^{-iak_z} \\
\alpha\, \mathrm{e}^{-iak_z} & \varrho_\alpha & \alpha\, \mathrm{e}^{iak_z} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \alpha\, \mathrm{e}^{-iak_z} & \varrho_\alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
- & - & - & - & - & - & - & - & - & - \\
0 & 0 & 0 & \varrho_\alpha & \alpha\, \mathrm{e}^{iak_z} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \mathrm{e}^{-iak_z} & \varrho_\alpha & \mathrm{e}^{iak_z} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \mathrm{e}^{-iak_z} & \varrho_\beta & \mathrm{e}^{iak_z} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \beta\, \mathrm{e}^{-iak_z} & \varrho_\beta & 0 & 0 & 0 \\
- & - & - & - & - & - & - & - & - & - \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \varrho_\beta & \beta\, \mathrm{e}^{iak_z} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta\, \mathrm{e}^{-iak_z} & \varrho_\beta & \beta\, \mathrm{e}^{iak_z} \\
\mathrm{e}^{iak_z} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta\, \mathrm{e}^{-iak_z} & \varrho_\beta
\end{array}\right]_{n_a+n_b}
\tag{9}
$$

where: $\varrho_\alpha = \dfrac{\hbar\omega - \Delta}{W} + \alpha F$, $\varrho_\beta = \dfrac{\hbar\omega - \varepsilon\Delta}{W} + \beta F$. Unknown $n_a + n_b$ Green's functions can be found as $G_{n_l;m_l} = \dfrac{D_{n_l;m_l}}{D}$, where $D_{n_l;m_l}$ is variable determinant, while D is system determinant. The calculation of Green's function poles, which define the spectrum of possible electron energies, turns into calculation of the roots of the system determinant, i.e.:

$$D = \alpha^{(n_a+n_b)}\mathcal{P}_{n_a}(\frac{\varrho}{\alpha})\mathcal{P}_{n_b}(\frac{\varrho}{\alpha}) - 2\alpha^{(n_a+n_b-2)}\mathcal{P}_{n_a-1}(\frac{\varrho}{\alpha})\mathcal{P}_{n_b-1}(\frac{\varrho}{\alpha}) + \quad (10)$$
$$+ \alpha^{(n_a+n_b-4)}\mathcal{P}_{n_a-2}(\frac{\varrho}{\alpha})\mathcal{P}_{n_b-2}(\frac{\varrho}{\alpha}) + (-1)^{(n_a+n_b+1)}\alpha^{(n_a+n_b-2)}\ 2\cos\left[(n_a+n_b)ak_z\right] = 0\ ,$$

where $\mathcal{P}_n$ are Chebishev's type polynomials [8]. Condition (10) is written for simple superlattice formed of super-layers of identical atoms ($\Delta^a = \Delta^b = \Delta$ and $W^a = W^b = W$), while energy transfer between the super-layers is different ($W \neq \tilde{W}$). In general case this condition can be solved only numerically. Various combinations of super-layers numbers (n_a and n_b) and electron transfer energies (W and $\tilde{W}$) were analyzed. The numerical results for $k_x = k_y = 0$ are graphically presented on Fig.2 and Fig.3.

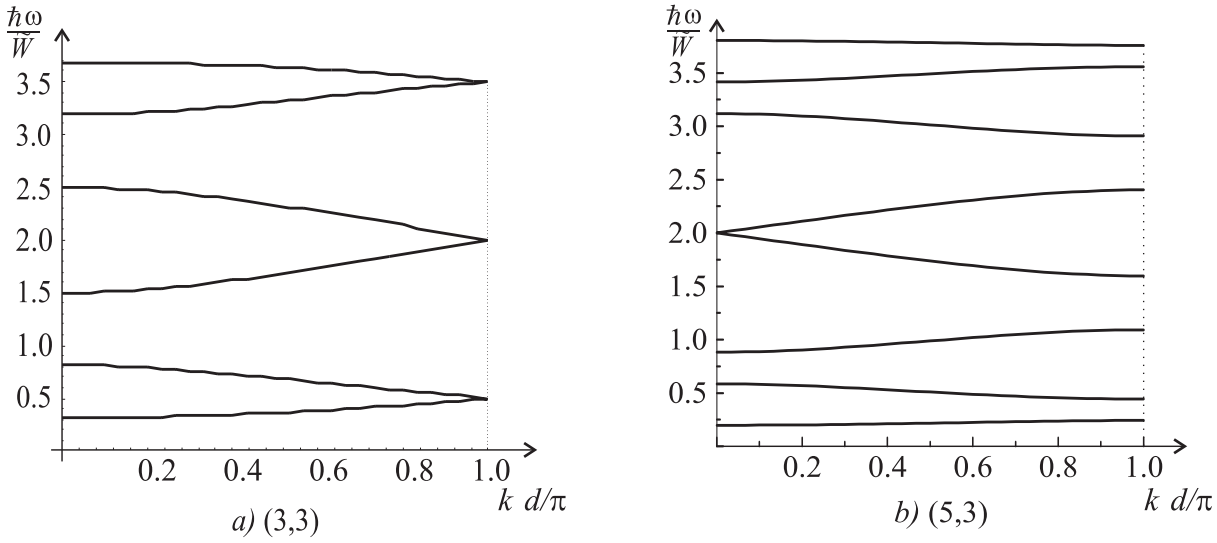

Figure 2: Electron dispersion law for $W = 0.5\tilde{W}$

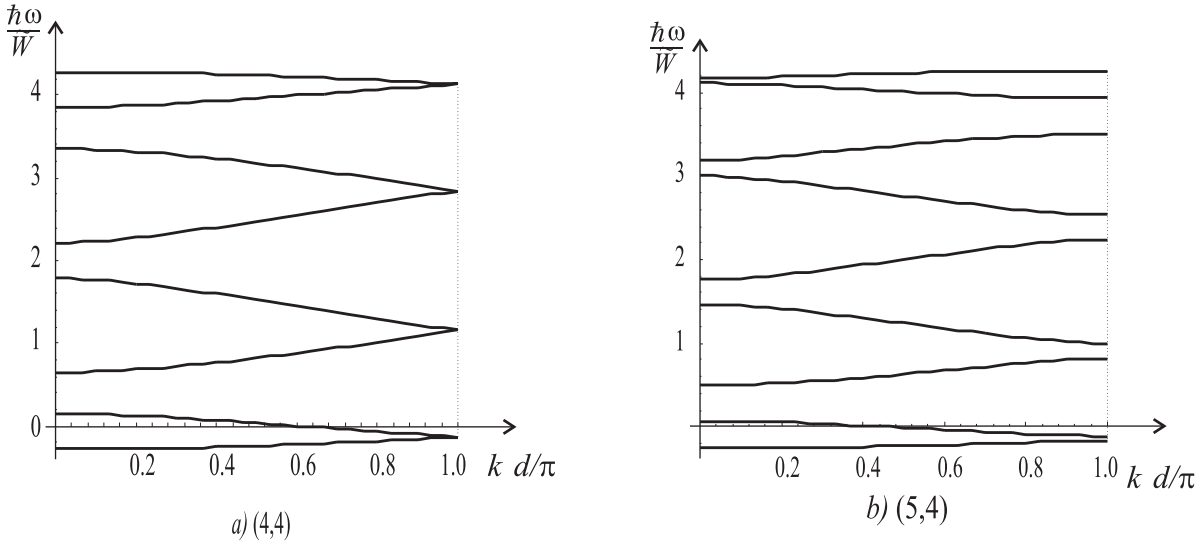

Figure 3: Electron dispersion law for $W = 1.5\tilde{W}$

Due to new periodicity along z-direction electron dispersion curve of superlattice splits into several ($n_a + n_b = d$) quasi-continual dispersion branches separated by forbidden bands. If energy transfer between super-layers is weaker than inside them ($W < \tilde{W}$) all allowed energy bands lie inside bulk energy limits ($\hbar\omega/\tilde{W} \in [0, 4]$), i.e. the superlattice energy zone becomes narrower (Fig.2). In analogy with thin film model [7,8], we can say that bottom and top energy gap appear. That is direct consequence of the decreasing of electron transfer between super-layers. Superlattice energy zone spreads outside the bulk energy limits when energy transfer $W > \tilde{W}$. Energy mini-bands of localized electron states appear (Fig.3). In variance to the crystalline film [7], where exist discrete localized states, mini-bands of localized states in superlattice are quasi-continual, due to infinity of superlattice.

Position, as well as distribution of energy mini-bands depends on number of layers and electron energy transfer. In the case of symmetrical superlattices ($n_a = n_b$), with identical atoms ($a = b$), energy mini-bands join at the end of the first Brillouin zone. The change of electronic transfer between identical symmetrical super-layers does not lead to opening of forbidden zones for $k_z = \pi/(n_a + n_b)\tilde{a}$ [6,10]. Superlattice parameter is: $(n_a + n_b)/2 = n_a$, because both of super-layers have the same length. If central mini-bands join at the edge or at centre of Brillouin zone electron dispersion law has a symmetry trough the line $\hbar\omega/\tilde{W} = 2$ (Fig 2b). Symmetry trough the point $k_z = \dfrac{\pi}{2\tilde{a}(n_a + n_b)}, \dfrac{\hbar\omega}{\tilde{W}} = 2$ (Fig 3b) appears when mini-bands are not joined [6].

3 Spectral weights and spatial distribution

Space distribution of electrons can be found by layer's spectral weights of Green's functions [9,11]. The starting point is the system of equations for Green's functions (8), written in matrix form: $\hat{\mathcal{D}}\tilde{\mathcal{G}} = \tilde{\mathcal{K}}$, where $\hat{\mathcal{D}}$ is $n_a + n_b$ order system matrix, while $\tilde{\mathcal{G}}$ and $\tilde{\mathcal{K}}$ are Green's functions and "right hand side" vectors [11]. Applying inverse matrix $\hat{\mathcal{D}}^{-1}$ we get: $\tilde{\mathcal{G}} = \hat{\mathcal{D}}^{-1}\tilde{\mathcal{K}}$, i.e:

$$G_{n_l;m_l} = \frac{1}{D}\sum_q D_{n_l;q_l}\mathcal{K}_{q_l;m_l} = \frac{1}{D}\frac{i\hbar}{2\pi W}\sum_q D_{n_l;q_l}\delta_{q_l;m_l} \ . \tag{11}$$

$D_{n_l;q_l}$ being co-factors of system matrix. We calculated only diagonal Green's functions $G_{n_l;n_l}$, due to their importance in equilibrium processes. Factorizing multi-pole functions [9,11] we obtain:

$$G_{n_l;n_l} = \frac{i\hbar}{2\pi W}\sum_{\nu=1}^{n_a+n_b}\frac{g_{n_l;n_l}(\varrho_\nu)}{\varrho - \varrho_\nu} \ . \tag{12}$$

The spectral weights $g_{n_l;n_l}(\varrho)$ are given by:

$$g_{n_l;n_l}(\varrho) = \frac{D_{n_l;n_l}(\varrho_\nu)}{\dfrac{d}{d\varrho}D(\varrho)|_{\varrho=\varrho(\nu)}} \tag{13}$$

Spectral weights represent squared moduli of wave function and enable us to analyze spatial distribution of finding electrons along superlattice layers (z direction). By numerically analyzes we calculate spectral weights of electrons for above mentioned simple superlattices (Fig.4).

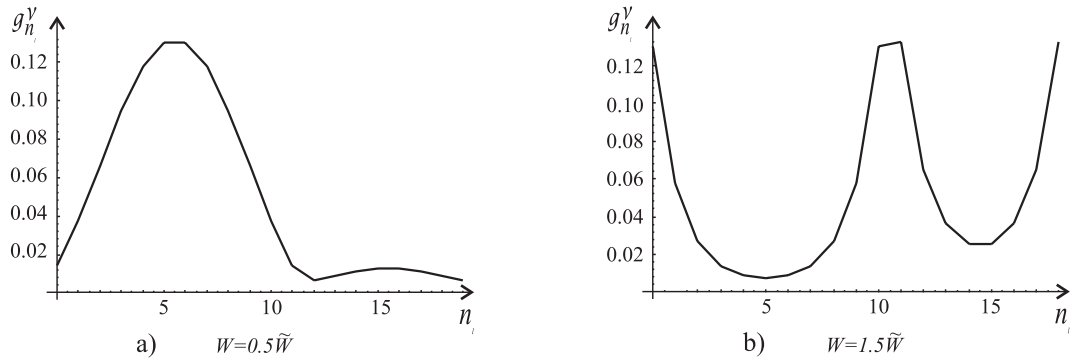

Figure 4: Space distribution of electron in superlattice

If $W < \tilde{W}$ all states are bulk (Fig 4a), while for $W > \tilde{W}$ localized states can appear (Fig. 4b). Some bulk states are distributed equally in both of material, but states of lowest and highest energies are distributed only in one of material. Space distribution depends on number of layers of superlattice. For even number of layers (dispersion law has symmetry trough the line $\hbar\omega/\tilde{W} = 2$) there is the symmetry of space distribution (for lowest and highest energies etc.) Localized states appear in centre of Brillouin zone if $W > \tilde{W}$, but in edge just for enough value of $W/\tilde{W}$. For odd number of layers (symmetry of dispersion law trough point $(k_z = \pi/(2a(n_a + n_b)), \hbar\omega/\tilde{W} = 2)$) there is symmetry between centre and edge of Brillouin zone and localized states appear always when $W > \tilde{W}$ [11]. Localized states appear, mostly, on higher energies. By increasing ratio $W/\tilde{W}$ number of these states increase.

4 Conclusion

In this paper we applied Green's function method in order to study electron configuration of superlattices. Apart from electron dispersion law and spectral weights, calculated here, this approach enables the consistent derivation of some other statistical characteristics values of superlattices (thermodynamics, transport, dielectric and other physical properties). Analyzing electron spectra and states of electrons in superlattice we obtain the following results:

1. An infinite superlattice separates free electron continuum onto allowed extended states and forbidden bands, as a results of new periodicity of superlattice, as well as changed electron transfer between super-layers.
2. All mini-bands lie inside bulk energy limits when energy transfer of electrons between super-layers is weaker than inside them, so bottom and top energy gaps appear. These typical bulk states can be distributed only in one of the films, what is shown by analysis of spatial distribution of electrons.
3. Superlattice energy zone spreads outside bulk energy limits when electron energy transfer between super-layers stronger than inside them. Energy mini-bands of localized states appear. Probability of finding an electron in these states is the maximal in the boundary layers with sharp decrease inside layers.

The interest to described nanostructures in material science is based on the possibility of manipulation of the physical properties of materials and devices by changing of mentioned

characteristic parameters (number of layers and electron energy transfer). On the basic this model and applied method there is possibility to investigate some other models of superlattice, such as aperiodic (Fibonacci) superlattice with a novel physical properties [12].

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