NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2011, 2 (4), P. 32–50

UDC 517.958

LANDAU-ZENER EFFECT FOR A QUASI-2D PERIODIC SANDWICH

N. Bagraev[1], G. Martin[2], B. S. Pavlov[2,3], A. Yafyasov[3]

[1]A. F. Ioffe Physico-Technical Institute, Russian Academy of Sciences, St. Petersburg, Russia
[2]NZ Institute for Advanced study, Massey University, Albany Campus, New Zealand
[3]V. Fock Institute for Physics at Physical Faculty of the St. Petersburg University, Russia

bagraev@mail.ioffe.ru, g.j.martin@massey.ac.nz,
pavlovenator@gmail.com, yafyasov@desse.phys.spbu.ru

Bloch-waves in 1D periodic lattices are typically constructed based on the transfer-matrix approach, with a complete system of solutions of the Cauchy problem on a period. This approach fails for the multi-dimensional Schrödinger equations on periodic lattices, because the Cauchy problem is ill-posed for the associated elliptic partial differential equations. In our previous work [8] we suggested a different procedure for the calculation of the Bloch functions for the 2D Schrödinger equation based on the Dirichlet-to-Neumann map substituted for the transfer -matrix. In this paper we suggest a method of calculation of the dispersion function and Bloch waves of quasi-2D periodic lattices, in particular of a quasi-2D sandwich, based on construction of a fitted solvable model.

Keywords: Landau-Zener effect, Bloch waves.

1. Transfer- matrix and DN-map approach to construction of Bloch- functions in 1D periodic lattices

The study of the basic quantum features of solids can be reduced to the one-body spectral problem on periodic lattices and construction of the quasi-periodic solutions of the one-body Schrödinger equation - Bloch-functions, see [16, 19]. In the 1D case Bloch-functions are constructed on the period $(0, a)$, $q(x + a) = q(x)$, as linear combinations $\chi = \theta + m\varphi$ of standard solutions of the Cauchy problem satisfying the initial conditions $\theta(0) = 1, \theta'(0) = 0,\ \varphi(0) = 0, \varphi'(0) = 1$:

$$-\theta'' + q\theta = \lambda\theta,\ -\varphi'' + q\varphi = \lambda\varphi \tag{1}$$

A linear combination $\chi = \theta + \mu\varphi$ of the two above solutions, with Wronskian equal to 1, represents a *Bloch function*, if it satisfies the quasi-periodic boundary conditions

$$\chi(a) = \mu\chi(0),\ \chi'(a) = \mu\chi'(0).$$

The corresponding spectral bands σ_s are defined by the condition $-1 \leqslant \mathcal{T}/2(\lambda) \leqslant 1$ imposed on the trace $\mathrm{Tr}\,\mathcal{T}(\lambda) = [\theta(a) + \varphi'(a)$ of the transfer matrix

$$\mathcal{T} = \begin{pmatrix} \theta(a) & \varphi(a) \\ \theta'(a) & \varphi'(a) \end{pmatrix} :\ \mathcal{T}\begin{pmatrix} u(0) \\ u'(0) \end{pmatrix} = \begin{pmatrix} u(a) \\ u'(a) \end{pmatrix} = \mu \begin{pmatrix} u(0) \\ u'(0) \end{pmatrix}.$$

In fact the Bloch solution $\chi(x, p)$ is bounded on the real axis x, if $p^2 = \lambda$ is on the spectral bands and does not tend to zero at infinity , $|x| \to \infty$, that is only if $\mu = e^{ipa}$, with real quasi-momentum p.

In particular for the Bloch solution $\chi = \theta + m\varphi$ we have

$$\mathcal{T}\begin{pmatrix} 1 \\ m \end{pmatrix} = \mu \begin{pmatrix} 1 \\ m \end{pmatrix}.$$

Thus the Cauchy data $(1, m)$ of the Bloch function give an eigenvector of the transfer matrix with the eigenvalue μ :

$$\det \begin{pmatrix} \theta(a) - \mu & \varphi(a) \\ \theta'(a) & \varphi'(a) - \mu \end{pmatrix} = 0$$

thus $\mu^2 - [\theta(a) + \varphi'(a)]\, \mu + 1 = 0$.

Hence the dispersion $\lambda = \lambda(p)$ and the position of the spectral bands $\sigma : |\mu| = 1$ are defined by the trace of the transfer matrix, see Fig.1.

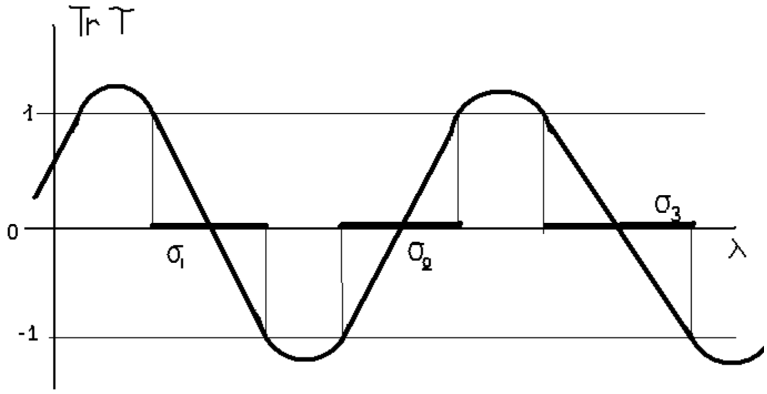

Fig. 1. The spectral bands σ_s of the 1D periodic problem found from the condition $-1 \leqslant \mathrm{Tr}\ \mathcal{T} < 1$.

The above "transfer-matrix path" to the construction of Bloch functions fails in the case of multi-dimensional periodic lattices, because the Cauchy problem is ill-posed for these elliptic PDEs. Fortunately this is not the only way to calculate the dispersion function and the Bloch waves, even in the 1D case.

Indeed, we can obtain Bloch solutions from an analysis of a boundary problem, by consider, instead of the standard solutions θ, φ of the Cauchy problem, another pair of solutions ψ_0, ψ_a of the same Schrödinger equation $-\psi'' + q\psi = \lambda\psi$, with the boundary data $\psi_0(0) = 1, \psi_0(a) = 0$ and, respectively $\psi_a(0) = 0, \psi_a(a) = 1$, see Fig. 1 (1,2) below. These solutions ψ_0, ψ_a of the Schrödinger equation are linearly independent if λ is not an eigenvalue of the corresponding Dirichlet problem on the period.

$$W(\psi_0, \psi_a)\Big|_0 = -{\psi_a}'(0) = W(\psi_0, \psi_a)\Big|_a = {\psi_0}'(a) = W(\psi_0, \psi_a)\Big|_a .$$

Then the Bloch solution can be found as a linear combination of ψ_0, ψ_a in the form

$$\chi(x) = \chi(0)\psi_0(x) + \chi(a)\psi_a(x) = \chi(0)\left[\psi_0(x) + e^{ipa}\psi_a(x)\right] \tag{2}$$

which implies:

$$\chi'(a) = \chi(0)\left[\psi_0'(a) + e^{ipa}\psi_a'(a)\right] = e^{ipa}\,\chi(0)\ \left[\psi_0'(0) + e^{ipa}\psi_a'(0)\right].$$

Eventually, the quasi-momentum exponential $e^{ipa} = \mu$ will be found from the quadratic equation

$$[\psi_0'(a) + \mu\psi_a'(a)] = \mu\ [\psi_0'(0) + \mu\psi_a'(0)]$$

which can be re-written as

$$\mu^2 + \frac{\psi_0'(0) - \psi_a'(a)}{\psi_a'(0)}\,\mu - \frac{\psi_0'(a)}{\psi_a'(0)} = \mu^2 + \frac{\psi_0'(0) - \psi_a'(a)}{\psi_a'(0)}\,\mu + 1 = 0. \tag{3}$$

Here the coefficient in front of $-\mu$ is equal again to trace Tr $\mathcal{T} = \mu + \mu^{-1}$ of the transfer-matrix:

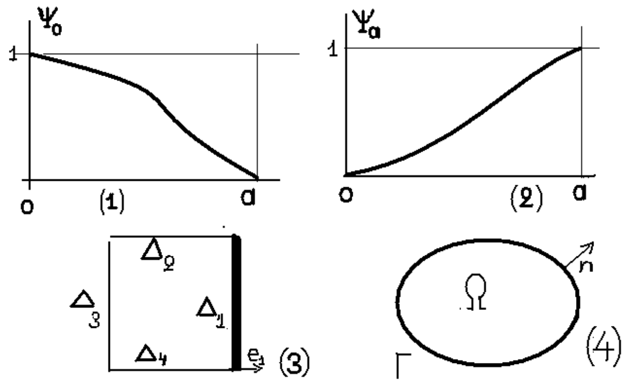

Fig. 2. Standard solutions ψ_0 (1) of the 1D boundary problem. Standard solutions ψ_{Δ^1} of the 2D boundary problem on the square period (3). Standard solutions of the boundary problems on the domain with a smooth boundary (4).

Thus the Bloch solution can be constructed of the standard solutions ψ_0, ψ_a as $\chi(0)[\psi_0 + \mu\psi_a]$.

This naive approach to the construction of the Bloch function, contrary to previous, based on the transfer matrix, can be extended to multidimensional lattices, because it is dealing with objects naturally defined in a multidimensional environment. Indeed, define the Dirichlet-to-Neumann map (DN-map) as the transformation of the Diricjhlet boundary data $\psi(0), \psi(a)$ of the solution ψ on the boundary into the Neumann data $\psi'(0), \psi'(a)$, associated with the positive direction on the x-axis. Notice, that our definition of the 1D DN - map, in this section, is only slightly different from the standard one which is associated with the positive normal on the boundary of the domain, but not with the positive direction of the x-axis :

$$\mathcal{DN}_{stand}\begin{pmatrix} u(0) \\ u(a) \end{pmatrix} \equiv \begin{pmatrix} -u'(0) \\ u'(a) \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} u'(0) \\ u'(a) \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}\mathcal{DN}\begin{pmatrix} u(0) \\ u(a) \end{pmatrix}$$

Hence our DN-map transfers the Dirichlet data $(u(0), u(a))$ as follows:

$$\begin{pmatrix} \psi_0'(0) & \psi_a'(0) \\ \psi_0'(a) & \psi_a'(a) \end{pmatrix}\begin{pmatrix} u(0) \\ u(a) \end{pmatrix} = \begin{pmatrix} u'(0) \\ u'(a) \end{pmatrix} \equiv \mathcal{DN}\begin{pmatrix} u(0) \\ u(a) \end{pmatrix}. \tag{4}$$

Then the quasi-periodic conditions imposed onto the boundary data $(1, \mu)\chi(0), (1, \mu)\chi'(0)$ of the Bloch function are represented as a homogeneous equation with respect to the the independent variables $(u(0), u'(0))$:

$$\begin{pmatrix} \psi_0'(0) & \psi_a'(0) \\ \psi_0'(a) & \psi_a'(a) \end{pmatrix}\begin{pmatrix} 1 \\ \mu \end{pmatrix}\chi(0) = \begin{pmatrix} 1 \\ \mu \end{pmatrix}\chi'(0) \tag{5}$$

This can be considered as a homogeneous equation for Cauchy data $(\chi(0), \chi'(0))$ at the left border point $x = 0$ of the period. Then a nonzero solution of the problem exists under the determinant condition.

$$\det\begin{pmatrix} \psi_0'(0) + \mu\psi_a'(0) & -1 \\ \psi_0'(a) + \mu\psi_a'(a) & -\mu \end{pmatrix} = 0,$$

which coincides with (3).

This approach is based on the boundary problem and the Dirichlet-to-Neumann map, see next section for it's two-dimensional version. The Cauchy problem is present here just in the form of the data $(u(0), u'(0))$, which can be considered as independent coordinates characterizing the solution u, due to the uniqueness theorem: $(u(0) = 0, u'(0) = 0$ involves vanishing of the corresponding solution of the Schrödinger equation $-u'' + qu - \lambda u = 0)$.

2. DN-map approach to construction of Bloch- functions in quasi-2D periodic lattices

The proposed method of constructing of Bloch functions does not rely on the existence of solutions of the Cauchy problem. Instead, it uses the uniqueness of the solution of the Cauchy problem and the Dirichlet -to-Neumann map. Both details are present in the multidimensional case, although the existence of solutions of Cauchy problems is not guaranteed. Fortunately we do not need the existence here.

Really the only difference between the general multidimensional approach suggested from the one-dimensional version is the unified choice of the direction of the direction of the normal derivative on the boundary: the positive normal is defined in multidimensional case as an exterior normal, which involves changing signs of some matrix elements of the DN-map.

In the multidimensional case the roles of the basic solutions ψ_0, ψ_a of the boundary problems for the Schrödinger equation on the square 2D period are played by solutions associated with the boundary data forming an orthogonal basis $\{\psi_s^\Gamma\} \in L_2(\Gamma)$ on the boundary of the period $\Omega : \partial\Omega = \Gamma$, see Fig.2, (4):

$$-\triangle \psi_s + q\psi_s = \lambda\psi_s,\ \psi_s\Big|_\Gamma = \psi_s^\Gamma,\ \langle\psi_s^\Gamma, \psi_t^\Gamma\rangle_{L_2(\Gamma)} = \delta_{st}.$$

Due to the uniqueness theorem for these elliptic equations the solutions $\{\psi_s\}$ are linearly independent, and their linear combinations approximate a solution of any boundary problem with the boundary data u_Γ decomposed on the boundary basis.

This fact allows us to define and calculate the Dirichlet-to-Neumann map on the domain as an operator in the space of boundary values of smooth solutions transforming the Dirichlet boundary data u_Γ into the Nemann boundary data - the normal derivatives

$$\mathcal{DN} : u_\Gamma \longrightarrow \frac{\partial u}{\partial n}\Big|_\Gamma, \tag{6}$$

see [23] for a discussion of the appropriate Sobolev classes. To calculate the matrix of the DN-map with respect to an orthogonal basis $\{u_s\}$ on the smooth boundary Γ, consider the matrix element of the DN-map

$$\int_\Gamma \bar{u}_l\, \frac{\partial u_m}{\partial n} d\Gamma \equiv \langle u_l, \mathcal{DN} u_l\rangle$$

Then the Green's formula allows us to transform the matrix element into the bilinear form of the Schrödinger operator.

$$\langle u_l, \mathcal{DN} u_m\rangle = \int_\Omega \left[\nabla\bar{u}_l \nabla u_m + q\bar{u}_l\, u_m - \lambda\bar{u}_l\, u_m\right] d\Omega. \tag{7}$$

This formula now allows us to calculate effectively the trace of the DN-map in some finite-dimensional subspaces, if the spectral parameter λ is far from the eigenvalues of the Dirichlet problem on the domain Ω. When λ is close to a Dirichlet eigenvalue , it is more convenient to calculate the matrix elements of the Neumann-to-Dirichlet map. This is done based on the same formula (7), but beginning from the solution of a sequence of Neumann problems for a smooth orthogonal basis $\{\rho_s\}$ in $L_2(\Gamma)$

$$-\triangle v_s + q v_s = \lambda v_s,\ \frac{\partial v_s}{\partial n}\Big|_{\Gamma} = \rho_s.$$

Then the Green formula implies the following expression for the matrix elements of the Neumann-to-Dirichlet map

$$-\triangle v + qv - \lambda u,\ \mathcal{ND} : \frac{\partial u}{\partial n}\Big|_{\Gamma} \longrightarrow v\Big|_{\Gamma}.$$

$$\langle \mathcal{ND}\rho_l, \rho_m\rangle = \int_{\Omega} \left[\nabla \bar{v}_l \nabla v_m + q\bar{v}_l\, v_m - \lambda \bar{v}_l\, v_m\right] d\Omega. \tag{8}$$

Once the Neumann-to-Dirichlet map is constructed, the Dirichlet-to-Neumann map, should it exist for given λ, can be obtained as the inverse of the former, $\mathcal{DN}\,\mathcal{ND} = I$.

Notice, that the DN map , associated with the outward positive normal, has a negative imaginary part in the upper halfplane $\Im\lambda > 0$, but the inverse $\mathcal{ND}$ is a Nevanlinna-class function. Obviously choosing the inward positive normal results in $\mathcal{ND}$ with the negative imaginary part and the Nevallinna-class operator function $\mathcal{DN}$.

Consider the quasi- 2D periodic lattice with a cubic period, see Fig. 3, and the Schrödinger operator

$$Lu = -\triangle u + q(x)u \tag{9}$$

on the lattice, with periodic potential $q(x^1, x^2) = q(x^1 + ma, x^2 + na)$, $m, n = \pm 1, \pm 2, \dots$, zero boundary conditions on the lower and the upper lids $\Gamma^3_0 : x^3 = 0$, $\Gamma^3_h : x^3 = h$ of the lattice.

In this way the whole spectral problem on the lattice is reduced to the spectral problem on the period, with the same boundary conditions on the lids $\Gamma^3_{0,h}$, and the quasi-periodic conditions on the vertical walls $\Gamma^{1,2}_{0,a}$.

The positive normal on $\Gamma^{1,2}_a$ is defined by e_1, e_2, and the positive normals on the walls $\Gamma^{1,2}_0$ are $-e_1, -e_2$. The quasi-periodic boundary conditions permit us to eliminate the boundary data $u\big|_{\Gamma^{1,2}_0}, \frac{\partial u}{\partial n}\big|_{\Gamma^{1,2}_0}$ on the walls $\Gamma^{1,2}_0$:

$$u\Big|_{\Gamma^{1,2}_0} = e^{-ip_{1,2}a} u\Big|_{\Gamma^{1,2}_a}, \qquad \frac{\partial u}{\partial n}\Big|_{\Gamma^{1,2}_0} = -e^{-ip_{1,2}a}\frac{\partial u}{\partial n}\Big|_{\Gamma^{1,2}_a}.$$

Then the quasi-periodic boundary conditions on the walls $\Gamma^{1,2}_{0,a}$ are reduced to a linear system with respect to the "independent variables" $\vec{u} = (u^1_a, u^2_a; \frac{\partial u}{\partial n}\Big|_{\Gamma^1_a}, \frac{\partial u}{\partial n}\Big|_{\Gamma^2_a})$, with a matrix composed of the components of the $\mathcal{DN}$ on the walls:

$$\begin{pmatrix} \frac{\partial u}{\partial n}\Big|_{\Gamma^1_0} \\ \frac{\partial u}{\partial n}\Big|_{\Gamma^2_0} \\ -e^{-ip_{1,2}a}\frac{\partial u}{\partial n}\Big|_{\Gamma^1_a} \\ -e^{-ip_{1,2}a}\frac{\partial u}{\partial n}\Big|_{\Gamma^2_a} \end{pmatrix} \equiv \begin{pmatrix} \frac{\partial \vec{u}_a}{\partial n} \\ -\mu^{-1}\frac{\partial \vec{u}_a}{\partial n} \end{pmatrix} = \mathcal{DN} \begin{pmatrix} u\Big|_{\Gamma^1_a} \\ u\Big|_{\Gamma^2_a} \\ e^{-ip_1 a}u\Big|_{\Gamma^1_a} \\ e^{-ip_2 a}u\Big|_{\Gamma^2_a} \end{pmatrix} \tag{10}$$

$$\mathcal{DN}\begin{pmatrix} u\Big|_{\Gamma_a^1} \\ u\Big|_{\Gamma_a^2} \\ e^{-ip_1 a}u\Big|_{\Gamma_a^1} \\ e^{-ip_2 a}u\Big|_{\Gamma_a^2} \end{pmatrix} \equiv \mathcal{DN}\begin{pmatrix} \vec{u}_a \\ \mu^{-1}\vec{u}_a \end{pmatrix}. \tag{11}$$

Here $\mu = [\mu_1, \mu_2] = [e^{1p_1 a}, e^{1p_2 a}]$ is a diagonal matrix. The DN-map $\mathcal{DN}$ can be represented in matrix form with 2×2 blocks $\mathcal{DN}^{ik}_{\alpha\beta}$ connecting the Dirichlet data on Γ^k_β to the Neumann data on Γ^i_α.

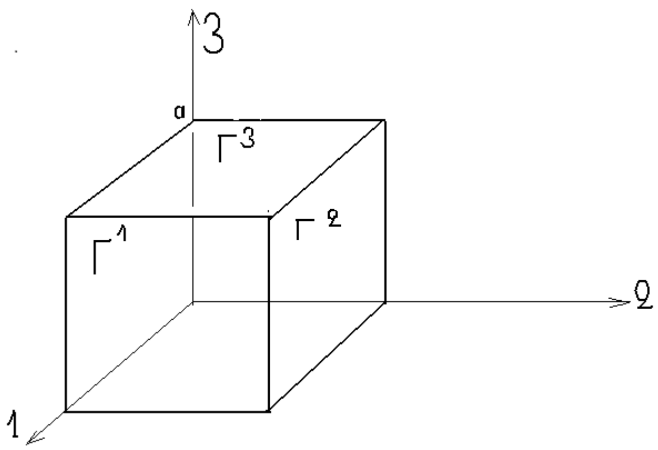

Fig. 3. 3D-period of the quasi-2D lattice, with zero boundary conditions on Γ^3_α.

Matrix elements of the DN map connect the Dirichlet data on Γ^{ik}_α with Neumann data on $\Gamma^{jl}_{\alpha'}$.

$$\begin{pmatrix} \mathcal{DN}^{11}_{aa} & \mathcal{DN}^{12}_{aa} \\ \mathcal{DN}^{21}_{aa} & \mathcal{DN}^{22}_{aa} \end{pmatrix} \equiv \mathcal{DN}_{aa}, \begin{pmatrix} \mathcal{DN}^{11}_{a0} & \mathcal{DN}^{12}_{a0} \\ \mathcal{DN}^{21}_{a0} & \mathcal{DN}^{22}_{a0} \end{pmatrix} \equiv \mathcal{DN}_{a0}.$$

$$\begin{pmatrix} \mathcal{DN}^{11}_{0a} & \mathcal{DN}^{12}_{0a} \\ \mathcal{DN}^{21}_{0a} & \mathcal{DN}^{22}_{0a} \end{pmatrix} \equiv \mathcal{DN}_{0a}, \begin{pmatrix} \mathcal{DN}^{11}_{00} & \mathcal{DN}^{12}_{00} \\ \mathcal{DN}^{21}_{00} & \mathcal{DN}^{22}_{00} \end{pmatrix} \equiv \mathcal{DN}_{00}.$$

Then the DN-map is represented by the block-matrix

$$\mathcal{DN} = \begin{pmatrix} \mathcal{DN}_{aa} & \mathcal{DN}_{a0} \\ \mathcal{DN}_{0a} & \mathcal{DN}_{00} \end{pmatrix}.$$

with blocks mapping the data $\vec{u}_a$, $\vec{u}_0$ onto the positive normal derivatives $\frac{\partial \vec{u}_a}{\partial n}, \frac{\partial \vec{u}_0}{\partial n}$. In particular, the 0-components of the Bloch function can be eliminated based on $\vec{u}_0 = \mu^{-1}\vec{u}_a$, $\frac{\partial \vec{u}_0}{\partial n} = \mu^{-1}\frac{\partial \vec{u}_a}{\partial n}$, which implies the following linear homogeneous system for the data $\left(\vec{u}_a, \frac{\partial \vec{u}_a}{\partial n}\right)$ of the Bloch -function:

$$\begin{pmatrix} \frac{\partial \vec{u}_a}{\partial n} \\ -\mu^{-1}\frac{\partial \vec{u}_a}{\partial n} \end{pmatrix} = \begin{pmatrix} \mathcal{DN}_{aa} & \mathcal{DN}_{a0} \\ \mathcal{DN}_{0a} & \mathcal{DN}_{00} \end{pmatrix} \begin{pmatrix} \vec{u}_a \\ \mu^{-1}\vec{u}_a \end{pmatrix}. \tag{12}$$

Eliminating $\frac{\partial \vec{u}_a}{\partial n}$ we conclude that a nontrivial solution of the equation (12) exists if and only if zero is an eigenvalue of the operator:

$$[\mu \mathcal{DN}_{0a}\mu + \mu \mathcal{DN}_{00} + \mathcal{DN}_{aa}\mu + \mathcal{DN}_{00}]\, \vec{u}_a = 0. \tag{13}$$

Then the Bloch function is obtained as a solution of the boundary problem for the Schrödinger equation

$$-\triangle \chi + q\chi = \lambda\chi.\ \chi\Big|_{\Delta_a^{1,2}} = u_a^{1,2},,\ \chi\Big|_{\Delta_0^{1,2}} = e^{-ip_{1,2}a}\ u_a^{1,2}.$$

Equation (13) is an analog of the quadratic equation (3), however questions concerning the existence of the corresponding solution of it in the general case is not yet completely understood, because we can't use the classical determinant condition of existence of non-trivial solutions of the homogeneous equation (13), see analysis of a general situation based on Schur complement - a matrix analog of the determinant "— in [18].

Fortunately for us, the physically meaningful spectral problem on the cubic periodic lattice with romboidal periods and relatively narrow connecting channels Γ_α^i, $\alpha = 0, a; 1 = 1, 2$, gives a chance of simplification of the model down to the solvable level.

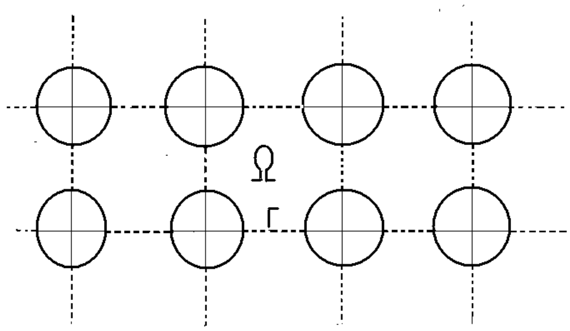

Fig. 4. 2D periodic lattice with romboidal periods

3. Finite-dimensional low-energy approximation for the dispersion surface of a quasi-2D periodic lattice

The structure of branches of the wave-functions on the links, connecting neighboring periods is determined mainly by the eigenfunctions of the conductivity band and by the covalent bonds formed from the upper filled orbitals on the period. Lower orbitals are essentially localized inside the period. This observation suggests that we substitute the spectral problem on the whole periodic lattice by one supplied with additional "partial" zero boundary conditions on the contacts Γ_α^i of the neighboring periods applied on the orthogonal complement $N^\perp \subset L_2(\Gamma)$ of the *contact space* N and the partial matching of eigenfunctions of the valent and conductivity bands on N :

$$P^N u\Big|_{\Gamma_0^l} = e^{-ip_l a} P^N u\Big|_{\Gamma_0^l};\ P^N \frac{\partial u}{\partial n}\Big|_{\Gamma_0^l} = -e^{-ip_l a} P^N \frac{\partial u}{\partial n}\Big|_{\Gamma_a^l};\ P_N^\perp u\Big|_{\Gamma_{0,a}^l} = 0. \tag{14}$$

The structure of the corresponding spaces $N, N^\perp$ depends on the energy, however for low temperature the energy is defined by the Fermi level Λ_F of the material and thus, in this regime, N can be selected independently of the energy. Then the above boundary conditions (14) define, together with the potential q and the corresponding differential expression $Lu = -\triangle u + qu$, a selfadjoint operator L_N on the period, with *partial quasi-periodic* boundary condition in $N \subset L_2(\Gamma)$. In fact the contact space N is the main parameter of our one-body model of the 2D periodic lattice. The freedom of choice of N here can be used in different ways to understand the structure and the functioning of the valent bonds and conductivity in solids.

The DN-map of the model Schrödinger equation with Dirichlet zero boundary condition on the complementary subspace and partial Dirichlet boundary condition in the contact space N

$$-\triangle u + qu = \lambda u, P_N^{\perp} u\Big|_{\Gamma^l} = 0,\ P^N u\Big|_{\Gamma^l} = u_\Gamma^N \in N. \tag{15}$$

is obtained via framing of the standard DN-map by the projections P^N onto the contact space N of the covalent bonds and conductivity channels.

$$\mathcal{DN}^N \equiv P^N \mathcal{DN} P^N.$$

Then the dispersion equation of the model with a chosen contact space N is obtained, as in (13), via substitution of the standard DN-map by the partial DN map

$$\left[\mu \mathcal{DN}_{0a}^N \mu + \mu \mathcal{DN}_{00}^N + \mathcal{DN}_{aa}^N \mu + \mathcal{DN}_{00}^N\right] \vec{u}_a = 0. \tag{16}$$

The ultimate equation, contrary to (13), is finite-dimensional. This allows us to obtain the dispersion equation for the model periodic quasi-2D lattice in explicit form as a determinant condition of existence of a nontrivial solution of the homogeneous equation. Indeed, assume that there exist a single resonance eigenvalue of the relative Dirichlet problem, situated close to the Fermi level Λ^F, $\lambda_1^D \approx \Lambda^F$, on the period, with an eigenfunction φ_1^D. Then, for low temperature, the relative DN-map can be replaced on the temperature interval near the Fermi level $\left(\Lambda^F - 2m\kappa T\hbar^{-2}, \Lambda^F + 2m\kappa T\hbar^{-2}\right)$ by a sum of a one-dimensional polar term and a correcting term

$$\mathcal{DN}^N \approx \frac{P^N \frac{\partial \varphi_1^D}{\partial n}\rangle \langle P^N \frac{\partial \varphi_1^D}{\partial n}}{\lambda - \lambda^1} + P^N B P^N \equiv \frac{Q^N}{\lambda - \lambda_1} + B^N.$$

Hence (16) is represented in a matrix form, based on the decomposition $N = \sum_{i=1,2,\alpha=0,a} N(\Gamma_\alpha^i)$. Elimination of the variable $P^N \frac{\partial v}{\partial n}\Big|_{\Gamma_a}$ gives a *finite-dimensional* equation for $P^N v\Big|_{\Gamma_a}$ similar to one above, see (13)

$$\begin{aligned}&\left[\mu Q_{0a}^N \mu + \mu Q_{00}^N + Q_{aa}^N \mu + Q_{00}^N\right] \vec{u}_a + \\ &(\lambda - \lambda_1^D)\left[\mu B_{0a}^N \mu + \mu B_{00}^N + B_{aa}^N \mu + B_{00}^N\right] \vec{u}_a = 0,\end{aligned} \tag{17}$$

with $\mu = (\mu_1, \mu_2) = (e^{ip_1 a}, e^{ip_2 a})$. The determinant condition for existence of a non-trivial solution to the ultimate equation gives the dispersion equation $\lambda = \lambda(p_1, p_2)$ for the model Hamiltonian L_N of the periodic lattice.

4. Landau-Zener phenomenon and Bloch-functions on a quasi-2D periodic sandwich

The essence of the 1D Landau-Zener phenomenon is easy to see from the simplest example of two parallel strings

$$\frac{1}{c_1^2}\frac{\partial^2 u^1}{\partial t^2} = \frac{\partial^2 u^1}{\partial x^2} + \varepsilon u^2, \qquad \frac{1}{c_2^2}\frac{\partial^2 u^2}{\partial t^2} = \frac{\partial^2 u^2}{\partial x^2} + \varepsilon u^1,$$

manufactured from a magnetic material, weakly interacting due to their different or equivalent polarity. Re-writing the above linear system in terms of Fourier-dual variables τ, ξ (frequency and momentum) as

$$\frac{1}{c_1^2}\tau^2 \tilde{u}^1 = \xi^2 \tilde{u}^2 - \varepsilon \tilde{u}^2, \qquad \frac{1}{c_a^2}\tau^2 \tilde{u}^2 = \xi^2 \tilde{u}^1 - \varepsilon \tilde{u}^1$$

yields a dispersion equation in the form of a determinant condition for the Fourier-dual variables $p^2 = c^{-2}\tau^2 + \varepsilon^2$. The branches $\lambda_{1,2}(\varepsilon)$ of the dispersion curve $p = \lambda_{1,2}(\varepsilon)\tau$ are just straight lines crossing at the origin of the (τ, p) plane, but form two branches of a hyperbola for $\varepsilon > 0$. The Landau-Zener effect is precisely the transformation of the crossing of the terms $\lambda_1(p), \lambda_2(p)$

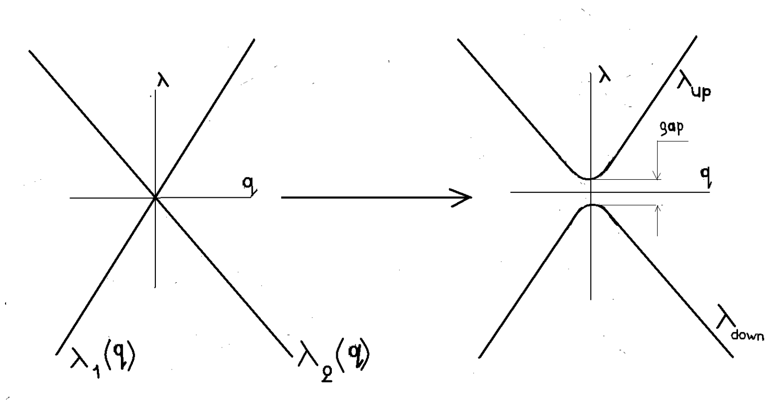

Fig. 5. One - dimensional Landau-Zener effect.

for $\varepsilon = 0$ into the "quasi-crossing" for $\varepsilon > 0$, as it is shown in Fig. 5 . This effect was first observed in [31], see an extended analysis of the 1D case in [12]. It was noticed that the interaction of terms λ_s in solid-state quantum problems leads to pseudo-relativistic properties of the corresponding particles/quasi-particles. Fresh interest for quasi-relativism in solid state physics arose in connection with the discovery of the high mobility of charge carriers in graphen, see for instance [13, 20, 28]. The 1D Landau-Zener effect in the case of weakly-interacting lattices can be considered as a "blowup" of the 0-dimensional singularity at the crossing point of the terms, see Fig.6 (1,2). Physicists have not yet decided on the magnitude of the mass of the charge carrier in Graphen, but there are recent theoretical indications, see [13], that it is small, but non-zero. This would mean that the conic dispersion surface presented in [20], may be interpreted a blowup of the tip of the cone, see Fig. 6 (3,4) Unfortunately, this hypothesis would contradict to our previous observations concerning the 2D Landau-Zener effect, see Fig. 8 (2). It remains an important question if an essential anisotropy of the effective mass of electron in graphen could be measured, to support the idea of the blowup resolution if the conic singularity presented on the picture in [20], but the mathematical arguments support the anisotropic stance of the resolution of the singularity on the line of intersection of two 2D terms blowing up in a form of a gutter, see Fig. 8 (2).

Indeed, the Bloch functions of two electrons on a pair of remoted periodic lattices with romboidal periods, see Fig 7, separated by a potential barrier (or two holes on lattices, separated by a quantum well) can be obtained as the product of the the Bloch functions on the isolated lattices. The corresponding dispersion equation for a single electron (hole) on the remoted lattices is obtained as a product of dispersion functions on the lattices $[E - E_u(\vec{p})][E - E_d(\vec{p})] = 0$. But if the mutual positions of the lattices permit the electron (hole) to jump from one lattice to another, then the product of the dispersion functions is transformed into the perturbed product $[E - E_u(\vec{p})][E - E_d(\vec{p})] = \varepsilon(E, \vec{p})$ with a small term in the right-hand side.

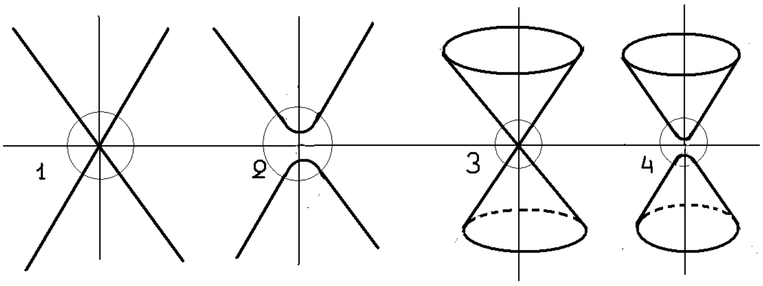

Fig. 6. The blowup of the zero-dimensional singularity for 1D terms (1,2) and 2D terms (3, 4)

Our aim is to calculate the perturbed equation based on the spectral data of the lattices and a model, see Fig. 8(1) of the interaction between lattices introduced via special assumptions about tunneling across the δ- barrier, see below. A naive physicist would easily see that the blowup of the intersection line of the dispersion surfaces $E = E_u(\vec{p}),\ E = E_d(\vec{p})$ of the upper and lower lattices with a barrier between them constitute a sandwich and would not give a cone (with a rounded top), see Fig. 8(4), but rather a gutter-like shape of the resulting dispersion surface, Fig. 8(3).

The final decision on the type of the blow-up (either the conic -like blowup or the gutter like blowup) must be recovered from experiments aimed at measurement of the effective mass anisotropy. But in this paper, based on our arguments above and also the modern analysis of blowup from 1D and 2D singularities in [24], we represent, see Fig. 8 (2), a theoretical analysis of the gutter-like blowup resolution of singularity localized of a curve obtained as an intersection of the 2D terms arising from the two neighboring periods of the upper and lower lattices of a quasi- 2D sandwich structure.

Our study is motivated by the recent discovery of the quasi-relativistic behavior of terms in the man-made sandwich of two periodic quasi-2D lattices, see [5]. We hope that the sandwich structures of two weak interacting quasi-periodic lattices can be used as a source of various artificial material structures with useful and interesting transport properties. The study of the Landau-Zener transformation in 2D case requires new analytic machinery, since, as we have noticed above, the 1D technique, based on the transfer-matrix, fails because of the "ill-posedness" of the Cauchy problem for Schrödinger equation on a square period. Thus we consider the periodic 2D sandwich based on Dirichlet-to-Neumann technique developed in the previous section.

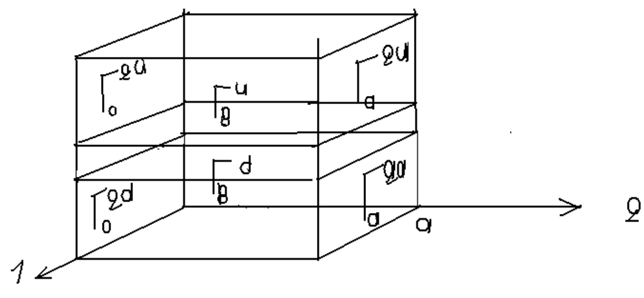

Fig. 7. Two-storied period of the periodic quasi-2D sandwich lattice

Originally we considered a 2-stordie period, see Fig. 7 with partial quasi-periodic boundary conditions on the vertical walls $\Gamma^{u,d}_{i,\alpha},\ 1 = 1, 2,\ \alpha = 0, a$, with the contact subspaces $N_{1,2}$, zero boundary conditions on the upper and lower lids Γ_h, Γ_{-h} and a bilateral potential barrier $\Gamma^{\pm}_b$, emulating the upper and lower layers of silicon heavily doped with borons and the intermediate layer of pure silicon, substituted by the δ-barrier.

This model is already soluble, but we make ome more step to obtain further simplification by substitution of the rectangular barrier by a δ- barrier, see Fig. 8(1). Denoting by $n_b^{d,u}$ the outer normals on both sides $\Gamma_b^{u,d}$ of the δ - barrier, we represent the boundary condition on Γ_b as

$$P_{N_b}\left[\frac{\partial \Psi^u}{\partial n^u}\Big|_{\Gamma_b^u} + \frac{\partial \Psi^d}{\partial n^d}\Big|_{\Gamma_b^d}\right] + \beta V_b = 0, \text{ with } \Psi_b = P_{N_b}\Psi^d\big|_{\Gamma_b^d} = P_{N_b}\Psi^u\big|_{\Gamma_b^u}. \tag{18}$$

Here we assume the continuity condition of the wave-function on the potential barrier and a jump of the normal derivative $\frac{\partial \Psi^u}{\partial n^u}\Big|_{\Gamma_b^u} + \frac{\partial \Psi^d}{\partial n^d}\Big|_b^d \equiv \left[\frac{\partial \Psi}{\partial n}\right]\Big|_{\Gamma_b}$ depending on the value of the N_b- projection $P_{N_b}\Psi^u\Big|_{\Gamma_b^u}$ of the wave-function on the barrier.

Once the magnitude of the tunneling constant β is fixed, we may consider the DN-map of the two-storied period with the joint vertical walls $\Gamma_{i,\alpha} = \Gamma_{i,\alpha}^u \cup \Gamma_{i,\alpha}^d$, and $N_i = N_i^u \cup N_i^d$. Then the dispersion equation for the 2D sandwich is similar to previous formulae (16,17).

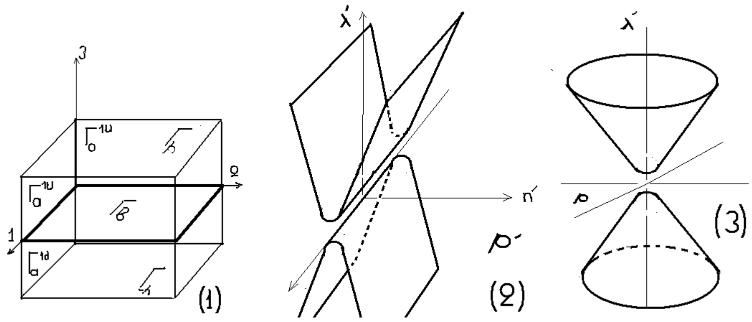

Fig. 8. Two-story period of the periodic quasi-2D sandwich lattice

It is interesting to observe the behavior of the dispersion surfaces in terms of the tunneling parameter β. To do this we consider the relative DN-maps of the upper and the lower stories Ω^u, Ω^d of the whole 2-story period Ω of the sandwich. Denote by N_1^u, N_i^d, N_b the contact subspaces associated with the corresponding walls $\Gamma_{\alpha,i}^u, \Gamma_{\alpha,i}^u, \Gamma_b$ and by $N_1^{u,\perp}, N_i^{d,\perp}, N_b^\perp$ the relevant orthogonal complements in the spaces of square-integrable functions on the walls.

$$\mathcal{DN}^u = \begin{pmatrix} \mathcal{DN}_{aa}^u & \mathcal{DN}_{a0}^u & \mathcal{DN}_{ab}^u \\ \mathcal{DN}_{0a}^u & \mathcal{DN}_{00}^u & \mathcal{DN}_{0b}^u \\ \mathcal{DN}_{ba}^u & \mathcal{DN}_{b0}^u & \mathcal{DN}_{bb}^u \end{pmatrix}, \tag{19}$$

with 2 blocks

$$\mathcal{DN}_{\alpha,\alpha'}^u = \begin{pmatrix} P_1^u \mathcal{DN}_{\alpha,\alpha'}^u P_1^u & P_1^u \mathcal{DN}_{\alpha,\alpha'}^u P_2^u \\ P_2^u \mathcal{DN}_{\alpha,\alpha'}^u P_1^u & P_2^u \mathcal{DN}_{\alpha,\alpha'}^u P_2^u \end{pmatrix}$$

and 2×1, 1×2 and 1×1 blocks

$$\mathcal{DN}_{\alpha,b}^u = \begin{pmatrix} P_1^u \mathcal{DN}_{\alpha,b}^u P_b^u \\ P_2^u \mathcal{DN}_{\alpha,b}^u P_b^u \end{pmatrix}, \ \mathcal{DN}_{b,\alpha}^u = \left(P_b^u \mathcal{DN}_{b\alpha}^u P_1^u; P_b^u \mathcal{DN}_{b,\alpha}^u P_2^u\right), \ \mathcal{DN}_{bb}^u = P_b^u \mathcal{DN}_{bb}^u P_b^u.$$

A similar representation is valid for $\mathcal{DN}^d$. The joint DN-map $\mathcal{DN}_{2D}$ of the period with continuity condition in N_b on Γ_b : $P_{N_b}\Psi\Big|_{\Gamma_b^u} \equiv P_b\Psi\Big|_{\Gamma_b^d}$ and the tunneling condition on the barrier

$$\left[P_b\frac{\partial\Psi}{\partial n}\right] + \beta P_b\Psi\Big|_{\Gamma_b} = 0$$

is given by the block-matrix acting on the vector $\left(\Psi_a^u, \Psi_0^u, P_b\Psi_b, \Psi_0^d, \Psi_a^d\right)$, with 2D components

$$\Psi_a^u \equiv (\Psi_{a1}^u, \Psi_{a2}^u),\ \Psi_0^u \equiv (\Psi_{01}^u, \Psi_{02}^u),$$

$$\Psi_a^d \equiv (\Psi_{a1}^d, \Psi_{a2}^u),\ \Psi_0^d \equiv (\Psi_{01}^d, \Psi_{02}^d)$$

and 1D component $P_b\Psi_b$.

$$\mathcal{DN}_{2D} = \begin{pmatrix} \mathcal{DN}_{aa}^u & \mathcal{DN}_{a0}^u & \mathcal{DN}_{ab}^u & 0 & 0 \\ \mathcal{DN}_{0a}^u & \mathcal{DN}_{00}^u & \mathcal{DN}_{0b}^u & 0 & 0 \\ \mathcal{DN}_{ba}^u & \mathcal{DN}_{b0}^u & \left[\mathcal{DN}_{bb}^u + \mathcal{DN}_{bb}^d\right] & \mathcal{DN}_{b0}^d & \mathcal{DN}_{ba}^u \\ 0 & 0 & \mathcal{DN}_{0b}^d & \mathcal{DN}_{00}^d & \mathcal{DN}_{0a}^d \\ 0 & 0 & \mathcal{DN}_{ab}^d & \mathcal{DN}_{a0}^d & \mathcal{DN}_{aa}^d \end{pmatrix}. \tag{20}$$

Due to the partial zero condition on the walls and the lids with selected contact subspaces $N_1^u, N_2^u, N_1^d, N_2^d, N_b$ of the open channels, the components of the boundary vectors are selected from these subspaces and the matrix elements are framed by projections onto $N_1^u, N_2^u, N_1^d, N_2^d, N_b$. We omit the projections in the formula (20) for the DN-map. The quasi-periodic boundary conditions are represented, with the diagonal matrices $\mu_u = [\mu_1^u, \mu_2^u]$ and $\mu_d = [\mu_1^d, \mu_2^d]$ on the boundary vectors, as

$$\mathcal{DN}_{2D} \begin{pmatrix} \Psi_a^u \\ \mu_u^{-1}\Psi_a^u \\ \Psi_b \\ \mu_d^{-1}\Psi_a^d \\ \Psi_a^d \end{pmatrix} = \begin{pmatrix} \frac{\partial V_a^u}{\partial n} \\ -\mu_u^{-1}\frac{\partial\Psi_a^u}{\partial n} \\ -\beta\,\Psi_b \\ -\mu_d^{-1}\frac{\partial\Psi_a^d}{\partial n} \\ \frac{\partial\Psi_a^d}{\partial n} \end{pmatrix} \tag{21}$$

The role of variables in these equations are played by the vectors $\Psi_a^u = (\Psi_{a1}^u, \Psi_{a2}^u) \in N_1^u \oplus N_2^u$, $\Psi_a^d = (\Psi_{a1}^d, \Psi_{a2}^d) \in N_1^d \oplus N_2^d$, $\frac{\partial\Psi_a^u}{\partial n} = (\frac{\partial\Psi_{a1}^u}{\partial n}, \frac{\partial\Psi_{a2}^u}{\partial n}) \in N_1^u \oplus N_2^u$, $\frac{\partial\Psi_a^d}{\partial n} = (\frac{\partial\Psi_{a1}^d}{\partial n}, \frac{\partial\Psi_{a2}^d}{\partial n}) \in N_1^u \oplus N_2^u$ and the vector $\Psi_b \in N_b$.

The vectors $\frac{\partial V_a^u}{\partial n}, \frac{\partial V_a^d}{\partial n}$ enter only into the right side of the last equation and can be easily eliminated, resulting in a homogeneous finite-dimensional linear system, which has a non-trivial solution under the determinant condition:

$$\det\begin{pmatrix} D_{11} & D_{12} & 0 \\ D_{21} & D_{22} & D_{23} \\ 0 & D_{32} & D_{33} \end{pmatrix} = 0 \tag{22}$$

, where

$$
\begin{aligned}
D_{11} &= \mathcal{DN}^u_{aa}\,\mu_u + \mathcal{DN}^u_{a0} + \mu_u\,\mathcal{DN}^u_{0a} + \mu_u\mathcal{DN}^u_{00},\\
D_{12} &= \mathcal{DN}^u_{ab} + \mu_d\,\mathcal{DN}^u_{0b},\\
D_{21} &= \mathcal{DN}^u_{ba}\mu_u + \mathcal{DN}^u_{b0},\\
D_{22} &= \mathcal{DN}^u_{bb} + \mathcal{DN}^d_{bb} + \beta I,\\
D_{23} &= \mathcal{DN}^d_{b0} + \mathcal{DN}^d_{ba}\mu_d,\\
D_{32} &= \mathcal{DN}^d_{ab} + \mu_d\,\mathcal{DN}^d_{0b},\\
D_{33} &= \mathcal{DN}^d_{aa}\,\mu_d + \mathcal{DN}^d_{a0} + \mu_d\,\mathcal{DN}^d_{0a} + \mu_d\mathcal{DN}^d_{00}.
\end{aligned}
$$

The determinant condition of existence of the nontrivial solution for large β takes the form:

$$
\begin{aligned}
&\det\left[\mathcal{DN}^u_{aa}\,\mu_u + \mathcal{DN}^u_{a0} + mu_u\,\mathcal{DN}^u_{0a} + \mu_u\mathcal{DN}^u_{00}\right] \times\\
\times &\det\left[\mathcal{DN}^d_{aa}\,\mu_d + \mathcal{DN}^d_{a0} + mu_d\,\mathcal{DN}^d_{0a} + \mu_d\mathcal{DN}^d_{00}\right] = O\left(\frac{1}{\det[\mathcal{DN}^u_{bb} + \mathcal{DN}^d_{bb} + \beta I]}\right),
\end{aligned}
\tag{23}
$$

gives a dispersion equation for the quasi-2D periodic sandwich for large β, which is represented as a blow-up of the crossing of 2D terms of the upper and lower planes of the sandwich :

$$
\begin{aligned}
&\det\left[\mathcal{DN}^u_{aa}\,\mu_u + \mathcal{DN}^u_{a0} + \mu_u\,\mathcal{DN}^u_{0a} + \mu_u\mathcal{DN}^u_{00}\right] \times\\
\times &\det\left[\mathcal{DN}^d_{aa}\,\mu_d + \mathcal{DN}^d_{a0} + \mu_d\,\mathcal{DN}^d_{0a} + \mu_d\mathcal{DN}^d_{00}\right] = 0.
\end{aligned}
\tag{24}
$$

Further simplification can be obtained via substitution of the matrix elements of $\mathcal{DN}_{2D}$ by the corresponding rational approximations near the resonance eigenvalues $\lambda^u_1, \lambda^d_1 \ldots$ of the partial Dirichlet problem, similar to (16, 17) in previous section. If there is only one simple resonance eigenvalue λ^u_1, λ^d_1 of the Schrödinger operator on each upper and low periods, then for the matrix elements of the upper and lower periods we have

$$
\mathcal{DN}^{u,d}_{\alpha,\alpha'} \approx \frac{Q^{u,d}_{\alpha,\alpha'}}{\lambda - \lambda^{u,d}_1} + B^{u,d}_{\alpha,\alpha'},
$$

which gives, due to finite dimension of the components, a rational equation for the dispersion function

$$
\begin{aligned}
&\det\left[Q^u_{aa}\,\mu_u + Q^u_{a0} + \mu_u\,Q^u_{0a} + \mu_u Q^u_{00} + (\lambda - \lambda^u_1)(B^u_{aa}\,\mu_u + B^u_{a0} + \mu_u\,B^u_{0a} + \mu_u B^u_{00})\right] \times\\
&\det\left[Q^d_{aa}\,\mu_d + Q^d_{a0} + \mu_d\,Q^d_{0a} + \mu_d Q^d_{00} + (\lambda - \lambda^d_1)(B^d_{aa}\,\mu_d + B^d_{a0} + \mu_d\,B^d_{0a} + \mu_d B^d_{00})\right] = O(\beta^{-1}),
\end{aligned}
$$

corresponding to the blowup of the intersection L of the dispersion surfaces of the upper and the lower components of the period. On a small neighborhood of a given point $(\lambda_l, \vec{p}_l \in L)$ of the intersection the blowup looks as a gutter oriented in the tangent direction of L, with curvature of the cross-section proportional to β, see Fig. 8(2). Thus the 2D Landau-Zener effect in the case of a sandwich defines a gutter- like dispersion surface, with a small effective mass in the direction orthogonal to the direction of the intersection L.

The practical receipt of construction of the dispersion surface for a two-storied quasi-2D lattice consists of several steps. Assuming that the two-storied period Ω is connected with neighboring ones by covalent bonds, we select the contact spaces $N_\Gamma \equiv N$ in a special way to reflect the structure of the covalent bonds on the boundary Γ of the period, and apply the partial zero boundary conditions on the orthogonal complements $N^\perp$ of N at the boundary of the periods. Select the basis in N_Γ and construct the partial DN and ND -maps in N for the Schrödinger operator on the period for a temperature interval of the spectral parameter close to the

Fermi level. Due to uniqueness theorem of the Cauchy problem for the Schrödinger equation, the difficulties in construction of the partial DN-map near the eigenvalues of the Dirichlet problem can be avoided via construction of the corresponding ND- map and using the connection between them $\mathcal{DN}\,\mathcal{ND} = I_N$. A one-pole (or, more generally, multi-pole) rational approximation of the DN-map on the energy interval near the Fermi level, taking into account the polar terms at the resonance eigenvalues on the interval and a regular approximation for the contribution from the complementary spectrum. This permits to find the finite-dimensional determinant condition of existence of nontrivial real quasimomenta and the corresponding "sandwich" Bloch functions obtained as a hybridization of the Bloch functions of the upper-lower layers of the sandwich.

5. Dispersion equation for a sandwich with a resonance barrier

More interesting physical picture arises when the barrier possess resonance properties, taken into account by the energy-dependence of the coefficient β, see [30]. The resonance properties may be caused by the size quantization on the space-charge region near the surface of the emitter, see for instance [29]. In the previous section we modeled a straight rectangular barrier by a δ barrier at the mutual boundary Γ_b of the upper and lower parts $\Omega^{u,d}$ of the two-storied period: $[\frac{\partial u}{\partial n}] + \beta u\Big|_{\Gamma_b} = 0$. In [7] the barrier has resonance properties defined by the sub-bands of 2D holes. Such a barrier can be modeled by the energy-dependent parameter β. This parameter arises in the course of the construction of a zero-range model of the resonance barrier. In this section we follow [21]when introducing the operator extension procedure for the finite positive matrix A - the inner Hamiltonian of the barrier

$$A = \sum_r \alpha_r^2\, P_r : E \to E,\, \dim E = n < \infty.$$

Here $\alpha_r^2 > 0$- the eigenvalues of the inner Hamiltonian of the barrier and $P_r = \nu_r\rangle\,\langle\nu_r$ are the corresponding orthogonal spectral projections. We will establish, as a result of our analysis, a duality between the eigenvalues and the dimension quantization levels, similar to the duality between the eigenvalues of the Dirichlet and Neumann problems on an interval. Restriction of the matrix A is equivalent to selection of the deficiency subspace for a given value of the spectral parameter. We choose the deficiency subspace $\mathcal{N}_i$ as a generating subspace of

$$A : \overline{\bigvee_{k>0} A^k \mathcal{N}_i} = E_A$$

such that

$$\frac{A+iI}{A-iI}\mathcal{N}_i \cap N_i = 0, \quad \dim \mathcal{N}_i = d.$$

Set

$$D_0^A = (A - iI)^{-1}\,(E_A \ominus \mathcal{N}_i)$$

and define the restriction of the inner Hamiltonian as $A \to A_0 = A\Big|_{D_0^A}$. Then $N_i \subset E_A$ plays the role of the deficiency subspace at the spectral point i, dim $\mathcal{N}_i = d$, $2d \leqslant$ dim E_A, and the dual deficiency subspace is $\mathcal{N}_{-i} = \frac{A+iI}{A-iI}\mathcal{N}_i$. The domain of the restricted operator A_0 is not dense in E_A, because A is bounded. Nevertheless, since the deficiency subspaces $\mathcal{N}_{\pm i}$ do not overlap, the extension procedure for the orthogonal sum $l_0 \oplus A_0$ can be developed, as in, for instance, [21]. In this case the "formal adjoint" operator for A_0 is defined on the defect $\mathcal{N}_i + \mathcal{N}_{-i} := \mathcal{N}$ by the von Neumann formula : $A_0^+ e \pm i\, e = 0$ for $e \in \mathcal{N}_{\pm i}$. Then the extension is constructed via restriction of the formal adjoint onto a certain plane in the defect where the boundary form vanishes (a

"Lagrangian plane"). According to the classical von Neumann construction all Lagrangian planes are parametrized by isometries $V : \mathcal{N}_i \to \mathcal{N}_i$ in the form

$$\mathcal{T}_V = (I - V)\mathcal{N}_i.$$

It follows from [21] that, once the extension is constructed on the Lagrangian plane, the whole construction of the extended operator can be finalized as a direct sum of the closure of the restricted operator and the extended operator on the Lagrangian plane.

Notice that the operator extension procedure may be developed without the non-overlapping condition also, see [17]. In particular, in the case $\dim E_A = 1$, which is not formally covered by the above procedure, was analyzed in [25] independently of [17]. The relevant formulas for the scattering matrix and scattered waves remain true and may be verified by direct calculation.

Choose an orthonormal basis in $\mathcal{N}_i$, say $\{f_s\}$, $s = 1, 2, \dots d$, as a set of deficiency vectors of the restricted operator A_0. Then the vectors $\hat{f}_s = \frac{A+iI}{A-iI} f_s$ form an orthonormal basis in the dual deficiency subspace $\mathcal{N}_{-i}$. Under the non-overlapping condition one can use the formal adjoint operator A_0^+ defined on the defect $\mathcal{N}$:

$$u = \sum_{s=1}^{d} [x_s\, f_s + \hat{x}_s\, \hat{f}_s] \in \mathcal{N}, \tag{25}$$

by the von Neumann formula, see [1],

$$A_0^+ u = \sum_{s=1}^{d} [-i\ x_s\, f_s + i\ \hat{x}_s\, \hat{f}_s]. \tag{26}$$

In order to use the symplectic version of the operator-extension techniques, we need to introduce in the defect a new basis $w_{s,\pm}$, on which the formal adjoint A_0^+ is correctly defined due to the non-overlapping condition above:

$$\begin{aligned} w_{s,+} &= \frac{f_s + \hat{f}_s}{2} = \frac{A}{A - iI} f_s \\ w_{s,-} &= \frac{f_s - \hat{f}_s}{2i} = -\frac{I}{A - iI} f_s, \end{aligned}$$

hence

$$A_0^+ w_{s,+} = w_{s,-} \qquad A_0^+ w_{s,-} = -w_{s,+}$$

It is convenient to represent elements $u \in \mathcal{N}$ via this new basis as

$$u = \sum_{s=1}^{d} [\xi_{+,s}\, w_{s,+} + \xi_{-,s}\, w_{s,-}]. \tag{27}$$

Then, using the notation $\sum_{s=1}^{d} \xi_{s,\pm}\, f_s := \vec{\xi}_\pm$ we re-write the above von Neumann formula as

$$u = \frac{A}{A - iI} \vec{\xi}_+^u - \frac{1}{A - iI} \vec{\xi}_-^u, \quad A_0^+ u = -\frac{1}{A - iI} \vec{\xi}_+^u - \frac{A}{A - iI} \vec{\xi}_-^u \tag{28}$$

The following formula for "integration by parts" for abstract operators was proved in [21].

Lemma 5.1. *Consider the elements u, v from the domain of the (formal) adjoint operator A_0^+:*

$$u = \frac{A}{A - iI} \vec{\xi}_+^u - \frac{1}{A - iI} \vec{\xi}_-^u, \ v = \frac{A}{A - iI} \vec{\xi}_+^v - \frac{1}{A - iI} \vec{\xi}_-^v$$

with coordinates $\vec{\xi}^u_{\pm}, \vec{\xi}^v_{\pm}$*:*

$$\vec{\xi}^u_{\pm} = \sum_{s=1}^{d} \xi^u_{s,\pm} f_{s,i} \in N_i, \ \vec{\xi}^v_{\pm} = \sum_{s=1}^{d} \xi^v_{s,\pm} f_s \in N_i.$$

Then, the boundary form of the formal adjoint operator is equal to

$$\mathcal{J}_A(u,v) = \langle A_0^+ u, v\rangle - \langle u, A_0^+ v\rangle = \langle \vec{\xi}^u_+, \vec{\xi}^v_- \rangle_N - \langle \vec{\xi}^u_-, \vec{\xi}^v_+ \rangle_N. \tag{29}$$

One can see that the coordinates $\vec{\xi}^u_{\pm}, \vec{\xi}^v_{\pm}$ of the elements u, v play the role of the boundary values similar to $\{U'(0), U(0), V'(0), V(0)\}$ for the Schrödinger equation $-U'' + VU = \lambda U$ on $(0, a)$. We call these *symplectic coordinates* for the elements u, v. The next statement, proved in [21], is the main detail of the fundamental Krein formula [1], for generalized resolvents of symmetric operators. In our situation it is used in the course of the calculation of the scattering matrix.

Lemma 5.2. *The vector-valued function of the spectral parameter*

$$u(\lambda) = \frac{A + iI}{A - \lambda I} \ \vec{\xi}^u_+ := u_0 + \frac{A}{A - iI}\vec{\xi}^u_+ - \frac{1}{A - iI}\vec{\xi}^u_-, \tag{30}$$

satisfies the adjoint equation $[A_0^+ - \lambda I]u = 0$*, and the symplectic coordinates* $\vec{\xi}^u_{\pm} \in \mathcal{N}_i$ *of it are connected by the formula*

$$\vec{\xi}^u_+ = P_{N_i} \frac{I + \lambda A}{A - \lambda I} \vec{\xi}^u_- \tag{31}$$

The matrix-function

$$P_{N_i} \frac{I + \lambda A}{A - \lambda I} P_{N_i} := \mathcal{M} : \mathcal{N}_i \to \mathcal{N}_i$$

has a positive imaginary part in the upper half-plane $\Im m\ \lambda > 0$ and serves an abstract analog of the celebrated Weyl-Titchmarsh function, see [1, 15]. It exists almost everywhere on the real axis λ with a finite number of simple poles at the eigenvalues α_r^2 of A. The boundary values $\xi^u_{\pm}$ of the solution u of the adjoint equation $[A^+ - \lambda I]u = 0$ are connected via the abstract Weyl-Titchmarsh function as

$$\xi_- = \mathcal{M}\xi_+. \tag{32}$$

We obtain the zero-range model the resonance barrier Γ_b imposing of elements $\Psi = \left(\psi^d, \psi^b, \psi^u\right)$, $\psi^d \in L_2(\Omega^d), \psi^b \in E, \psi^u \in L_2(\Omega^u)$ boundary conditions at the barrier Γ_b. In what follows we restrict our analysis to the case of a one-dimensional defect, $d = 1$, that is scalar $\xi_{\pm}, \mathcal{M}$ and the one-dimensional jump of the normal derivative $P_b \frac{\partial \Psi}{\partial n}$ at the barrier Then, following [29] a selfadjoint boundary condition at the barrier can be selected based on a choice of 3D complex vector $\vec{\beta} = (1, \beta, 1)$ defining the Datta-Das Sarma boundary condition at the barrier imposed on the partial boundary values $\Psi\big|_{\Gamma_b} = \left(\psi^d, \xi_+, \psi^u\right)$, $\Psi'\big|_{\Gamma_b} = \left(P_b \frac{\partial \psi^d}{\partial n}, \xi_+, P_b \frac{\partial \psi^u}{\partial n}\right)$, with the normal directed outside the barrier:

$$\Psi'\big|_{\Gamma_b} \perp \vec{\beta}, , \Psi\big|_{\Gamma_b} \parallel \vec{\beta}.$$

For the selected above vector parameter $\vec{\beta} = (1, \beta, 1)$ this boundary condition looks like the condition at the δ-barrier:

$$P_b \frac{\partial \psi^d}{\partial n\big|_{\Gamma_b^d}} + P_b \frac{\partial \psi^u}{\partial n\big|_{\Gamma_b^u}} + \bar{\beta}\xi_+ = 0, \ P_b \psi^d = P_b \psi^u = \beta^{-1}\xi_- \equiv \Psi_b. \tag{33}$$

Eliminating the inner components $\xi_\pm$ of the boundary values based on (32), we obtain the boundary condition imposed on the partial jump $P_b \frac{\partial \psi^d}{\partial n}\big|_{\Gamma_b^d} + P_b \frac{\partial \psi^u}{\partial n}\big|_{\Gamma_b^u} \equiv \left[\frac{\partial \Psi}{\partial n}\right]_b$ of the wave-function:

$$\left[P_b \frac{\partial \Psi}{\partial n}\right]_b + |\beta|^2 \mathcal{M}^{-1} P_b \Psi_b = 0. \tag{34}$$

The dispersion equation for the sandwich with a resonance barrier is obtained from 21 via replacement of β^2 by $|\beta|^2\mathcal{M}^{-1}$. In fact at each zero of $\mathcal{M}$ the corresponding dispersion surface endures Landau-Zener effect, because the crossing of 2D terms is , in fact, transformed into quasi-crossing. Hence the zeros of $\mathcal{M}$ play the role of resonance levels of the dimensional quantization. This defines the duality between the eigenvalues of the inner Hamiltonian of the barrier and the poles of $\mathcal{M}$ which appear as resonance peaks corresponding to the sub-bands of 2D holes, similar to the duality revealed in our paper [29]. One can see that the resonance peaks at the sub-bands are dual to the eigenvalues of the inner Hamiltonian, which can be interpreted as the dimensional quantization levels, similarly to [29].

Suggested approach to calculation of the dispersion function and the Bloch waves is naturally extended to multidimensional lattices and sandwiches and forms a convenient analytical base for relevant computing. We postpone description of the corresponding material to the oncoming publications.

6. Superconductivity in a quasi-2D periodic sandwich: Landau- Zener gap enhancement

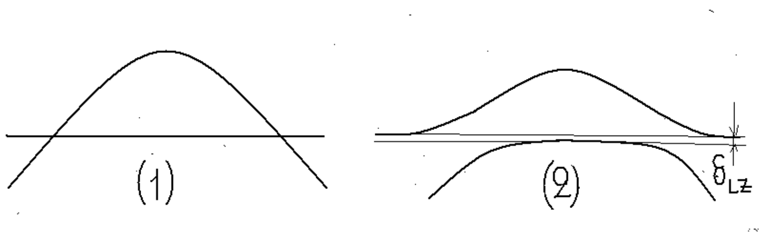

Fig. 9. Additional spectral gap arising from a simple and flat band overlapping: transformation of the band's crossing (1) into the quasi-crossing (2) (1D schematic figure)

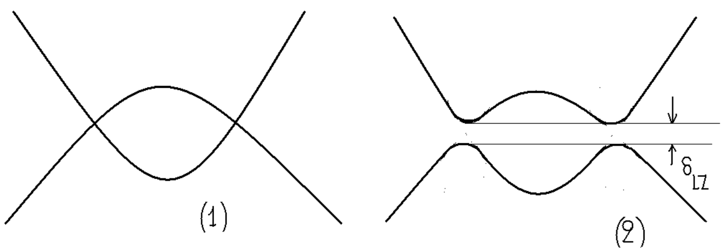

Fig. 10. Additional spectral gaps arising from the 2D Landau-Zener phenomenon: transformation of the crossing of the dispersion surfaces into the quasi-crossing (2) (the 2D section of the 3D gutter)

In [7] high-temperature superconductivity was observed in a Si-B sandwich. This is interpreted as a Josephson effect arising due to the interaction between the Bloch electrons on the upper and lower plates of the sandwich, defined by the boundary condition on the barrier Γ_b, see Fig. 10. The transformation of the crossing of the corresponding 2D terms into quasi-crossings — the Landau-Zener phenomenon — is similar to that discussed in [2] with the standard and flat bands overlapping, see Fig. 9. It was shown in [2] that in the one-dimensional model the spectral gap δ_{LZ}, arising due to the Landau-Zener phenomenon (Landau-Zener gap) causes the enhancement of the BCS gap and hence better high-temperature stability of the superconductivity phenomenon. In [7] additional electrodes were used to manipulate the positions of the sub-bands in the barrier, and the stable high-temperature conductivity effect was observed. The presence of the flat band is not essential for the theoretical interpretation of the superconductivity observed: the Landau-Zener gap arose due to the sandwich structure with a resonance barrier. But in the case [2] when the flat band is involved, the density of states $[\nabla_p \lambda]^{-1}$ is automatically large, while in the case of the SiB sandwich we do not have yet any theoretical estimation of the density of space to explain the HTSC effect. We hope to develop computing, based on above analysis, to obtain thew estimation in further publications.

7. Acknowledgement

Authors are grateful to the Marsden Fund of the Royal Society of New Zealand for a generous support which allowed the personal contacts of our team over the mountains and across the oceans.

One of authors (B.P.) is grateful to the Russian Academy for the support from the grant RFBR 03-01-00090.

References

[1] Akhiezer N.I., Glazman I.M. Theory of Linear Operators in Hilbert Space, Vol. 1. — New York: Frederick Ungar Publ., 1966. Translated from Russian by M. Nestel.

[2] Adamyan V., Pavlov B. High-Temperature superconductivity as a result of a simple and flat bands overlapping // Solid State Physics. — 1992. — V. 34, No. 2. — P. 626–635.

[3] Albeverio S., Gesztesy F., Hoegh-Krohn R., Holden H. Solvable models in quantum mechanics. — New York: Springer-Verlag, 1988.

[4] Albeverio S., Kurasov P. Singular Perturbations of Differential Operators. — London Math. Society Lecture Note Series, Vol. 271. — Cambridge University Press, 2000.

[5] Bagraev N., Buravlev A., Kljachkin L., Maljarenko A., Gehlhoff W., Romanov Yu., Rykov S. Local tunnel spectroscopy of silicon structures // Physics and Techniques of Semiconductors. — 2005. — V. 39, No. 6. — P. 716–727.

[6] Bagraev N., Mikhailova A., Pavlov B., Prokhorov L., Yafyasov A. Parameter regime of a resonance quantum switch // Phys. Rev. B. — 2005. — V. 71. — 165308, pp. 1–16.

[7] Bagraev N., Klyachkin L., Kudryavtsev A., Malyarenko A., Romanov V. Superconductor properties for silicon nanostructures // In: Superconductivity theory and application, Ed. by A. Luiz, SCIVO, Chapt. 4, 2010. — P. 69–92.

[8] Bagraev N., Martin G., Pavlov B. Landau-Zener Phenomenon on a double of weakly interacting quasi-2d lattices // In: Progress in Computational Physics: Wave propagation in periodic Media, Bentham Science publications (PiCP), 2010.01.06. — P. 61–64.

[9] Berezin F.A., Faddeev L.D. A remark on Schrödinger equation with a singular potential // Dokl. AN SSSR. — 1961. — V. 137. — P. 1011–1014.

[10] Brüning J., Martin G., Pavlov B. Calculation of the Kirchhoff coefficients for the Helmholtz resonator // Russ. J. Math. Phys. — 2009. — V. 16, No. 2. —P. 188–207.

[11] Callaway J. Energy band theory. — New York—London: Acacemic Press, 1964.

[12] Demkov Y.N., Kurasov P.B., Ostrovski V.N. Double-periodical in time and energy solvable system with two interacting set of states // J. Physics A, Math. General, **28** (1995) p.434.

[13] Firsova N., Ktitorov S. Electron's scattering in the monolayer graphen with the short range impurites // Phys. Letters A. — 2010. — V. 174. — P. 1270–1273.
[14] Fox C., Oleinik V., Pavlov B. A Dirichlet-to-Neumann approach to resonance gaps and bands of periodic networks // Proceedings of the Conference: Operator Theory and mathematical Physics, Birmingham, Alabama, 2005. In: Contemporary Mathematics. — 2006. — V. 412. — P. 151–169.
[15] Gorbachuk V.I., Gorbachuk M.L. Boundary value problems for operator differential equations // Translated and revised from the Russian, 1984. Mathematics and its Applications (Soviet Series), Vol. 48. Dordrecht: Kluwer Academic Publishers Group, 1991.
[16] Kittel C. Quantum Theory of Solids, Chapter 9. — New York—London: John Wiley & sons, inc., 1962.
[17] Krasnosel'skij M.A. On selfadjoint extensions of Hermitian Operators // Ukr. Mat. Zh. — 1949. — V. 1. — P. 21–38.
[18] Mennicken R., Shkalikov A. Spectral decomposition of symmetric operator-matrices // Mathematische Nachrichten. — 1996. — V. 179. — P. 259–273.
[19] Madelung O. Festkörpertheory. Bd. I, II, Ch. IV. — Berlin, Heidelberg, New York: Springer Verlag, 1972.
[20] Novoselov K., Geim A., Morozov S., Jiang D., Katsnelson I., Grigorieva I., Dubonos S. Two-dimensional gas of massless Dirac fermions in graphen // Nature. — 2005. — V. 438. — P. 197–200.
[21] Pavlov B. The theory of extensions and explicitly solvable models // Uspekhi. Mat. Nauk. — 1987. — V. 42, No. 6 (258). — P. 99–131.
[22] Pavlov B. The spectral aspect of superconductivity- the pairing of electrons // Vestnik Leningr. Uni. Math. Math. — 1987. — V. 3. — P. 43–49.
[23] Pavlov B. S-Matrix and Dirichlet-to-Neumann Operators // In: Encyclopedia of Scattering, ed. R. Pike, P. Sabatier, Academic Press, Harcourt Science and Tech. Company, 2001. — P. 1678–1688.
[24] Pospescu-Pampu P. Resolution of curves and surfaces // Lecture notes in Summer School of Resolution of Singularities, June 2006, Trieste, Italy.
[25] Shirokov J. Strongly singular potentials in three-dimensional Quantum Mechanics // Teor. Mat. Fiz. **42** 1 (1980) 45-49
[26] Sylvester J., Uhlmann G. The Dirichlet to Neumann map and applications // Proceedings of the Conference "Inverse problems in partial differential equations", Arcata, 1989. In: SIAM, Philadelphia. — 1990. — V. 101.
[27] Titchmarsh E.C. Eigenfunction expansion asociated with second -order differential equation, Part II, Chapter XXI. — Oxford at the clarendon press, 1958.
[28] Yafyasov A., Bogevol'nov V., Zelenin C. Manifestation of dimensional quantization of space-charge region of Carbon on differential capacitance and surface cons=ductivity measurements // Russian Academy Doklady, Electrochemie. — 1989. — V. 25. — P. 536–538.
[29] Yafyasov A., Bogevolnov V., Fursey G., Pavlov B., Polyakov M., Ibragimov A. Low-threshold emission from carbon nano-structures // Ultramicroscopy. — 2011. — V. 111. — P. 409–414.
[30] Yafyasov A., Martin G., Pavlov B. Resonance one-body scattering on a junction // Nanosystems: Physics, Chemistry, Mathematics. — 2010. — V. 1, No. 1. — P. 108–147.
[31] Zener C. Non-adiabatic crossing of energy levels. — Proc. Royal Soc. A. — 1932. — V. 137. — P. 696.
[32] Ziman J.,Mott N., Hirsch P. The Physics of Metals. — London, Cambridge, 1969.
[33] Ziman J. Electrons and phonons: the theory of transport phenomena in solids. — Oxford University Press, 1960.