

# Landau-Zener phenomenon on a sandwich of weakly interacting quasi-2d periodic lattices.

N. Bagraev <sup>1</sup>, G. Martin <sup>2</sup>, B. Pavlov <sup>2</sup>

<sup>1</sup>A.F. Ioffe Physico-Technical Institute, St. Petersburg, Russia,

<sup>2</sup>New Zealand Institute of Advanced Study, Massey University, New Zealand.

Isaac Newton Institute for Mathematical Sciences.  
Analysis on Graphs and its Applications Follow -up.  
26-30 July 2010

The dynamics of a single electron is considered on a periodic square 2d lattice constructed of rhomboidal quantum wells interacting via narrow links . The spectral structure of bands and gaps of the corresponding one-body Hamiltonian is derived from an accurate analysis of Bloch waves of a solvable model, constructed based on a rational approximation of DN- maps of the quantum wells by establishing a communication between them via partial boundary conditions emulating the covalent bonds. In the case of the corresponding sandwich of periodic lattice, the weak interaction of the two parallel periodic quasi-2d sub-lattices defines, due to the 2d Landau-Zener effect, a high mobility of the corresponding charge carriers in certain direction on the quasi-momenta plane.

# Introduction.

We start with comparison of mysteriously efficient coupled cluster approach to few-body problems in solid-state physics with a modified analytic perturbation procedure based on selection of the first order approximation. Transport properties of periodic lattices are defined by the structure of the corresponding Bloch eigenfunctions. In the 1d case the Bloch eigenfunctions are found based on the transfer matrix constructed of solutions of the relevant Cauchy problems. This approach fails in 2d, and, generally, in the multi-dimensional case, because the Cauchy problem for the multi-dimensional Schrödinger equation is ill-posed. The approach based on “tight binding” ideas (Linear Combination of Atomic Orbitals - LCAO , see [20, 21]), gives a reasonably good qualitative coincidence with experiment, but stays on a shaky mathematical basement.

# Introduction

The recent coupled cluster philosophy, see for instance [7] and references therein, gives a decisive hint for development an alternative approach to analysis of the Bloch functions in multidimensional periodic structures. Indeed, the periods of covalent crystals, sharing electrons, may play a role of *coupled clusters* - elementary blocks of the solid, connected by covalent bonds associated with certain partial summations of the perturbation series. An appropriate choice of the partial summations allows to emulate most essential details of the covalent bonds, see [10], of the neighboring clusters and thus can be interpreted as a substitution of the perturbed Hamiltonian by an appropriate solvable model which inherits most important spectral features of the perturbed Hamiltonian, see for instance [16], where only the coupled pairs of electrons are taken into account.

# Introduction

In this paper we consider first a simplest 2d square lattice with rhomboidal periods weakly connected with each other by the relatively narrow links. The wave-functions components supported by the links correspond to covalent bonds. The whole 2d crystal is considered as a periodic quantum network, with the Fermi-level situated on the conductivity band. In the case when the products  $K_- d_s$  of the exponents  $K_-$  of the evanescent waves and the lengths  $d_s$  of the connecting links are large, the matching of the evanescent waves generated by the neighboring clusters can be substituted, on the Fermi level, by the partial zero boundary conditions  $P_- \psi \Big|_{\Gamma} = 0$  imposed on the cross-sections  $\Gamma$  of the connecting links (the slots), with the projections  $P_-$  onto the entrance subspace  $E_-$  the closed channels. Vice versa, the most essential part of the interaction defined by the covalent bonds is caused by the matching of the wave-functions in the open channels, which correspond to the

# Introduction

We guess that a convenient and realistic solvable model of the interaction of the neighboring periods of the 2d lattice can be obtained based on the partial matching conditions

$P_+ \psi \Big|_{\Gamma^-0} = P_+ \psi \Big|_{\Gamma^+0}$ , with the complementary orthogonal projection  $P_+$  onto  $E_+ = L_2(\Gamma) \ominus E_-$ , taking into account only the oscillating waves with the spectral parameter  $\lambda = 2mE\hbar^{-2}$  situated inside the temperature interval  $\Delta_T = [\Lambda - \frac{2m\kappa T}{\hbar^2}, \Lambda - \frac{2m\kappa T}{\hbar^2}]$  centered at the (scaled) Fermi level  $\Lambda = 2mE_F\hbar^{-2}$  of the lattice. Thus the solvable model is defined by the choice of the entrance subspaces  $E_{\pm}$  of the open and closed spectral channels. Selection of an appropriate entrance (cross-section) subspaces  $E_{\pm}$  of the closed and open channels on the links is actually a freedom we can use to simplify the original problem of matching of all one-body orbitals of the neighboring clusters.

Though the above assumption concerning the configuration of the **links** already allows to develop an appropriate analytic perturbation technique for the single-particle spectral analysis on the corresponding quantum network, based on filtering properties of the narrow channels, see for instance [9], we make one more step toward a simpler model, by neglecting the length of the links, but assuming that the one-body spectral problem on the periodic network is considered with the partial matching on the entrance subspace of the open channels and zero boundary condition in the closed channels, imposed on the common boundary  $\Gamma_{\vec{l}} = \Gamma_{\vec{l}'} =: \Gamma$  of the neighboring periods  $\Omega_{\vec{l}}, \Omega_{\vec{l}'}$ :

$$-\Delta\psi_{\vec{l}} + V(x)\psi_{\vec{l}} = \lambda\psi_{\vec{l}}, \quad x \in \Omega_{\vec{l}},$$

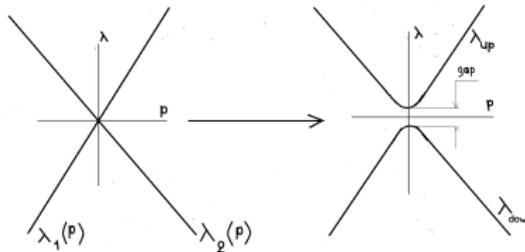
$$P_{-}\psi_{\vec{l}} \Big|_{\Gamma} = P_{-}\psi_{\vec{l}'} \Big|_{\Gamma} = 0,$$

$$P_{+}\psi_{\vec{l}} \Big|_{\Gamma} = P_{+}\psi_{\vec{l}'} \Big|_{\Gamma},$$

The operator defined on the quantum network  $U_T \Omega_T$  by (1) is self-adjoint and has a pure continuous spectrum. We guess that (1) takes into account an essential part of the interaction forming the Bloch-functions of the corresponding solvable perturbed Hamiltonian, defined by the selected from  $E_+$  cross-sections orbitals associated with the open channels on the links. Based on the model described, with use of the Dirichlet-to-Neumann map, see [18], we develop in this paper spectral analysis of the model 2d lattice from the first principles, and obtain the corresponding dispersion equations.

# Introduction

Based on results obtained for the 2d periodic lattice, we consider the corresponding sandwich of lattices assuming a weak interaction between the two sub-lattices. Considering the corresponding 2d Landau-Zener effect we conclude that the charge carriers dynamics on a two-layers periodic lattice may reveal some important features like high mobility in certain direction on the quasi-momenta plane.



**Figure:** One dimensional Landau-Zener effect.

# Introduction

It was observed first, see [19], in one-dimensional lattices, with use of the transfer-matrix as a main spectral tool for study of corresponding space or time- periodic structures, see [11]. It was noticed that the interaction of terms  $\lambda_s(p)$  in solid-state quantum problems implies pseudo-relativistic properties of the corresponding quasi-particles. Fresh interest for quasi-relativism in solid state physics arose in connection with discovery of high mobility of charge carriers in graphen, see for instance [15]. Recent discovery of quasi-relativistic behavior of terms in man-made bi-layer periodic quasi-2d lattices, see [2, 3], allows to conjecture that the weak interaction of 2d periodic lattices may be used as a source of various artificial structures with interesting transport properties. Study of the Landau-Zener transformation of 2d terms requires an adequate analytic machinery.

# Dispersion equation of the 2d lattice based on DN-map.

In [13] the Dirichlet-to-Neumann map was selected as an appropriate tool to substitute the transfer-matrix in analysis of perturbations of the two-dimensional terms. The standard DN-map is a linear transformation of the boundary “potential”  $\psi|_{\Gamma}$ ,  $\Gamma \subset \partial\Omega$  into the “boundary current”  $\frac{\partial\psi}{\partial n}|_{\Gamma}$  of the solution  $\psi$  of the homogeneous Schrödinger equation on the domain  $\Omega$ , with scaled spectral variable  $\lambda = \frac{2mE}{\hbar^2}$ .

$$-\Delta\psi + V\psi = \lambda\psi, \quad \mathcal{DN}(\lambda) : \psi|_{\Gamma} \longrightarrow \frac{\partial\psi}{\partial n}|_{\Gamma}.$$

In this paper we consider a modified version of DN-map, restricted by an orthogonal projection  $P_+$  onto entrance subspace  $E_+$  of the contact subspace  $L_2(\Gamma)$ .

# Dispersion equation of the 2d lattice based on DN-map.

We ignore the spin of electron and initially assume that the one-electron wave functions on the neighboring rhomboidal periods, see Fig. 3, communicate with each other via relatively narrow connecting channels, which filter the evanescent waves off, see an extended analysis of the filtering by narrow channels in [9].

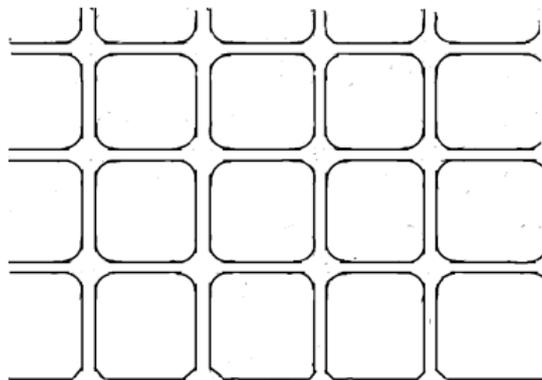
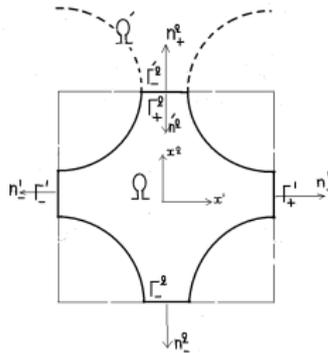


Figure: A general view of a lattice with rhomboidal periods.

The thresholds of the upper spectral bands containing the evanescent waves are situated above the Fermi level. The evanescent waves are filtered out.



**Figure:** A detail of a square lattice with rhomboidal periods. The connecting links are not shown.

# Dispersion equation of the 2d lattice based on DN-map.

We simplified the spectral problem via replacement of the matching condition on  $\Gamma$  in closed channels by the partial zero boundary condition on the slots  $\Gamma$ , see (1). The Schrödinger operator on the periodic lattice with above boundary conditions can be analyzed based on a quasi-periodic problem on the period, with the partial matching boundary condition substituted by the quasi-periodicity on the pairs of opposite slots  $\Gamma_{\pm}^s = \{x^s = \pm 1\}$  of the period  $\Omega$ :

$$\begin{aligned} P_+ \left[ \psi_{\Omega} \Big|_{\Gamma_-^s} \right] &= e^{-2ip_s a} P_+ \left[ \psi_{\Omega} \Big|_{\Gamma_+^s} \right], \\ P_+ \left[ \frac{\partial \psi_{\Omega}}{\partial n} \Big|_{\Gamma_-^s} \right] &= -e^{-2ip_s a} P_+ \left[ \frac{\partial \psi_{\Omega}}{\partial n} \Big|_{\Gamma_+^s} \right], \end{aligned} \quad (2)$$

where the differentiation is done with respect to the outward normals on the boundaries of the relevant periods, see Fig. (1). 

# Dispersion equation of the 2d lattice based on DN-map.

Hereafter we assume that the width  $2a = 2$  of the period is equal to 2,  $\delta/2 \ll 1$ , and the entrance subspace  $E_+^s$  of the open channel attached to each slot  $\Gamma_{\pm a}^s$  is one-dimensional and spanned by  $\sqrt{\frac{2}{\delta}} \sin \frac{\pi y}{\delta} = e^s$ ,  $P_+^s = e^s \langle e^s$  on each section  $\Gamma^s$ . The electron with the wave-function having a non-trivial boundary data on  $\Gamma^s = \partial\Omega \cap \partial\Omega'$  from common contact subspaces  $E^s = L_2(\Gamma^s)$  on the slots  $\Gamma_{\pm a}^s$  belongs to both periods and forms a covalent bond between the blocks  $\Omega, \Omega'$ . We use the relative intermediate DN-map  $\mathcal{DN}_\Gamma$  associated with spectral/boundary problems with partial data on the slots. Assuming that the neighboring periods are connected by the cylindrical links of certain width  $\delta$ , denote by  $P_\pm^s$  the projections onto the **cross-section (entrance) subspaces**  $E_\pm^s$  of the open and closed channels respectively.

# Dispersion equation of the 2d lattice based on DN-map.

We assumed that the Fermi-level is situated on the first spectral band  $\Lambda \in \Delta_1 = [\pi^2 \delta^{-2}, 4\pi^2 \delta^{-2}]$ , thus  $\Delta_1$  plays the role of the conductivity band. In fact, the Dirichlet Schrödinger operator on the period with zero boundary condition imposed onto the boundary values  $\psi \Big|_{\Gamma}$  is an intermediate Hamiltonian for the quasi-periodic problem with the boundary condition (1), obtained by formal setting the exponential in the closed channels as  $K_- = \infty$ , or, correspondingly, by choosing the above partial zero boundary conditions on the closed channels of the slots.

# Dispersion equation of the 2d lattice based on DN-map.

Then the corresponding DN-map  $\mathcal{DN}^\wedge$  for partial boundary values problem with  $P_+ u_\Gamma \in E_+$  is defined as a restriction of the standard DN-map onto the slots  $\Gamma$  with subsequent framing by the projections  $P_+ = \sum_{s=1,2,sgn} P_{sgn}^s$  onto  $E_+ = \sum_{s=1,sgn} E_{sgn}^1$ :

$$\begin{aligned}\mathcal{DN}^\wedge &= P_+ \mathcal{DN} P_+ \\ &= \sum_{s,t=1,2,sgn,sgn'} P_{sgn}^s \Big|_{\Gamma_{sgn}^s} \mathcal{DN} P_{sgn'}^t \Big|_{\Gamma_{sgn'}^t}.\end{aligned}$$

Hence the partial DN-map  $\mathcal{DN}^\wedge$  is defined by the matrix elements of the standard DN-map of the period in the decomposition of **the contact space**

$E = E_+ + E_- \equiv E = L_2(\Gamma)$  **of the slot**  $\Gamma$  into an orthogonal sum of the entrance subspaces of the open and closed channels.

# Dispersion equation of the 2d lattice based on DN-map.

We characterize the period  $\Omega$  on given spectral interval  $\Delta_T$  by the rational approximation with an appropriate correcting term

$$\mathcal{DN}^\wedge(\lambda) = \sum_{r=1}^n \frac{Q_r}{\lambda - \lambda_r} + P_+ K P_+, \quad \lambda_r \in \Delta_T, \quad (3)$$

where

$$\begin{aligned} & \frac{Q_r}{\lambda - \lambda_r} = \\ &= \sum_{s, \text{sgn}; t, \text{sgn}'} \langle \mathbf{e}_{\text{sgn}}^s \rangle \frac{\langle \mathbf{e}_{\text{sgn}}^s, \frac{\partial \psi_r}{\partial n} \rangle \langle \frac{\partial \psi_r}{\partial n}, \mathbf{e}_{\text{sgn}'}^t \rangle}{\lambda - \lambda_r} \langle \mathbf{e}_{\text{sgn}'}^t, \cdot \rangle \\ & P_+ K P_+ = \sum_{s, t, \text{sgn}, \text{sgn}'} \langle \mathbf{e}_{\text{sgn}}^s \rangle \langle \mathbf{e}_{\text{sgn}}^s K \mathbf{e}_{\text{sgn}'}^t \rangle \langle \mathbf{e}_{\text{sgn}'}^t, \cdot \rangle. \end{aligned} \quad (4)$$

Here  $\lambda_r$  are the eigenvalues of the Schrödinger operator with partial Dirichlet boundary conditions in closed channels on the essential spectral interval  $\Delta_+$  and  $P_+ K P_+$  - the restriction of the

# Dispersion equation of the 2d lattice based on DN-map.

The correcting term contains contributions to the DN - map from the complementary spectral subspace, corresponding to the eigenvalues on the complement of  $\Delta_T$ .

The spectral structure of the Schrödinger operator on the 2d periodic lattice is established based on study of the quasi-periodic spectral problem on the period  $\Omega$ , which is defined by the quasiperiodic boundary conditions connecting the projections of the boundary values and the boundary currents of the solutions of the Schrödinger equation  $L\psi = \lambda\psi$  on the opposite **slots**  $\Gamma_{\pm}^S$  of the period:

# Dispersion equation of the 2d lattice based on DN-map.

$$\begin{aligned} P_+ \begin{pmatrix} \psi_-^1 \\ \psi_+^1 \\ \psi_-^2 \\ \psi_+^2 \end{pmatrix} &= P_+ \begin{pmatrix} e^{-2ip_1} \psi_+^1 \\ \psi_+^1 \\ e^{-2ip_2} \psi_+^2 \\ \psi_+^2 \end{pmatrix} \\ &= \psi_+^1 \nu^1 + \psi_+^2 \nu^2, \\ P_+ \begin{pmatrix} \psi'_-{}^1 \\ \psi'_+{}^1 \\ \psi'_-{}^2 \\ \psi'_+{}^2 \end{pmatrix} &= P_+ \begin{pmatrix} -e^{-2ip_1} \psi'_+{}^1 \\ \psi'_+{}^1 \\ -e^{-2ip_2} \psi'_+{}^2 \\ \psi'_+{}^2 \end{pmatrix} \\ &= \psi'_+{}^1 \mu^1 + \psi'_+{}^2 \mu^2, \end{aligned} \tag{5}$$

# Dispersion equation of the 2d lattice based on DN-map.

where

$$\nu^1 = e^1 \begin{pmatrix} e^{-2ip_1} \\ 1 \\ 0 \\ 0 \end{pmatrix}, \nu^2 = e^2 \begin{pmatrix} 0 \\ 0 \\ e^{-2ip_2} \\ 1 \end{pmatrix},$$

$$\mu^1 = e^1 \begin{pmatrix} -e^{-2ip_1} \\ 1 \\ 0 \\ 0 \end{pmatrix}, \mu^2 = e^2 \begin{pmatrix} 0 \\ 0 \\ -e^{-2ip_2} \\ 1 \end{pmatrix},$$

and

$$\psi_+^s = \langle \psi \Big|_{\Gamma_{+a}^s}, \mathbf{e}^s \rangle, \psi'_+{}^s = \left\langle \frac{\partial \psi}{\partial n} \Big|_{\Gamma_{+a}^s}, \mathbf{e}^s \right\rangle.$$

# Dispersion equation of the 2d lattice based on DN-map.

Then the quasi-periodicity condition implies the equation:

$$\mathcal{DN}^\Lambda[\psi_+^1 \nu^1 + \psi_+^2 \nu^2] = \psi_+^{\prime 1} \mu^1 + \psi_+^{\prime 2} \mu^2, \quad (6)$$

with scalar coefficients  $\psi_+^s, \psi_+^{\prime 2}$ . Notice that  $\langle \nu^s, \mu^t \rangle = 0$ , which implies

$$\begin{aligned} \langle \nu^1 \mathcal{DN} \nu^1 \rangle \psi_+^1 + \langle \nu^1 \mathcal{DN} \nu^2 \rangle \psi_+^2 &= 0, \\ \langle \nu^2 \mathcal{DN} \nu^1 \rangle \psi_+^1 + \langle \nu^2 \mathcal{DN} \nu^2 \rangle \psi_+^2 &= 0 \end{aligned} \quad (7)$$

# Dispersion equation of the 2d lattice based on DN-map.

The condition of existence of the non-trivial Bloch function is represented in the determinant form:

$$\det \begin{pmatrix} \langle \nu^1, \mathcal{DN}_{11}\nu^1 \rangle & \langle \nu^1, \mathcal{DN}_{12}\nu^2 \rangle \\ \langle \nu^2, \mathcal{DN}_{21}\nu^1 \rangle & \langle \nu^2, \mathcal{DN}_{22}\nu^2 \rangle \end{pmatrix} = 0, \quad (8)$$

where  $\langle \nu^s, \mathcal{DN}_{st}\nu^t \rangle =$

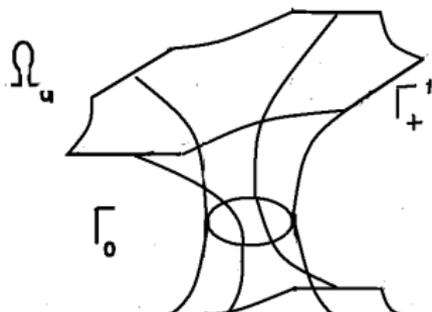
$$\sum_{r=1}^n \sum_{sgn, sgn'} \frac{\langle \nu^s \frac{\partial \psi_r}{\partial n} \rangle_{\Gamma_{sgna}^s} \langle \frac{\partial \psi_r}{\partial n}, \nu^t \rangle_{\Gamma_{sgn'a}^t}}{\lambda - \lambda_r} + \langle \nu^s, K\nu^t \rangle. \quad (9)$$

# Dispersion equation of the 2d lattice based on DN-map.

Of course all above constructions and arguments concerning 1d slots of 2d periods are automatically transferred to the case of 2d slots of the 3d periods of a quasi-2d lattice in  $R_3$ . We leave an exact formulation and verification of the corresponding wording to the reader, but just use it next section of our paper.

# Dispersion equation of a sandwich of quasi-2d lattice and 2d Landau-Zener effect.

We aim on the spectral analysis of a sandwich of periodic **quasi-2d** lattice with rhomboidal periods  $\Omega^u, \Omega^d$  playing the roles of basements of the upper and the lower cones of the two-storey joint period, see Fig.(4).



# Dispersion equation of a sandwich of quasi-2d lattice and 2d Landau-Zener effect.

Assume that first and the second storeys are connected by the link constructed in a form of adouble cone with the slot  $\Gamma_0$  dividing the upper and lower cones and a tunneling boundary condition on it defined by a real antisymmetric matrix

$$\mathbf{B} : P_0^\perp \psi^u \Big|_{\Gamma_0} = 0 = P_0^\perp \psi^d \Big|_{\Gamma_0} :$$

$$\begin{pmatrix} P_0 \frac{\partial \psi^u}{\partial n^u} \Big|_{\Gamma_0^u} \\ P_0 \frac{\partial \psi^d}{\partial n^d} \Big|_{\Gamma_0^d} \end{pmatrix} = \begin{pmatrix} 0 & -\beta \\ \beta & 0 \end{pmatrix} \begin{pmatrix} P_0 \psi^u \Big|_{\Gamma_0^u} \\ P_0 \psi^d \Big|_{\Gamma_0^d} \end{pmatrix}. \quad (10)$$

with the outward normals  $n^u = -n^d$ , and an orthogonal 1d projection  $P_0 = e^0 \rangle \langle e^0$  onto the open channels on the slot  $\Gamma_0^{u,d}$ .

# Dispersion equation of a sandwich of quasi-2d lattices and 2d Landau-Zener effect.

This tunneling boundary condition, with large  $\beta$ , emulates the potential barrier/well for the corresponding charge carriers (electrons/ holes, respectively) separating the upper and lower lattices, because implies  $\psi^u \approx 0 \approx \psi^d$  if  $\beta^{-1} \approx 0$ . If the slots  $\Gamma_{u,d}^s$  of the upper and lower periods are equipped with the matching boundary conditions on the contact with the neighboring periods, then the Schrödinger operator on the whole lattice, with a real, bounded and piecewise continuous periodic potential is selfadjoint, and the corresponding dispersion equation can be derived from the Bloch condition on a single period, via comparison of the boundary values

$$\vec{\Psi} = \left( \vec{\psi}_1^u, \vec{\psi}_2^u, \psi_0^u, \psi_0^d, \vec{\psi}_2^d, \vec{\psi}_1^d \right),$$

of the wave-functions on the slots  $\Gamma_u^s, \Gamma_0, \Gamma_d^t$  of the upper and lower periods and the balance of the corresponding boundary currents with the tunneling boundary condition

# Dispersion equation of the sandwich of quasi-2d lattices and 2d Landau-Zener effect.

Imposing the quasi-periodic boundary conditions on the slots  $\Gamma_{sgn a}^s(u)$ ,  $\Gamma_{sgn a}^s(d)$  and the tunneling boundary conditions on  $\Gamma_0^u$ ,  $\Gamma_0^d$ , we obtain the linear system for the variables  $\psi_+ = (\psi_{+a}^{u1}, \psi_{+a}^{2u}, \psi_0^u, \psi_0^d, \psi_{+a}^{u1}, \psi_{+a}^{u2})$ , similar to (8):

$$\langle \nu_u^1 \mathcal{DN}_{11}^u \nu_u^1 \rangle \psi_1^u + \langle \nu_u^1 \mathcal{DN}_{12}^u \nu_u^2 \rangle \psi_2^u + \langle \nu_u^1 \mathcal{DN}_{10}^u \rangle \psi_0^u = 0,$$

$$\langle \nu_u^2 \mathcal{DN}_{21}^u \nu_u^1 \rangle \psi_1^u + \langle \nu_u^2 \mathcal{DN}_{22}^u \nu_u^2 \rangle \psi_2^u + \langle \nu_u^2 \mathcal{DN}_{20}^u \rangle \psi_0^u = 0,$$

# Dispersion equation of a sandwich of quasi-2d lattice and 2d Landau-Zener effect.

$$\begin{aligned}\langle \mathcal{DN}_{01}^u, \nu_u^1 \rangle \psi_1^u + \langle \mathcal{DN}_{02}^u, \nu_u^2 \rangle \psi_2^u + \mathcal{DN}_{00}^u \psi_0^u &= -\beta \psi_0^d, \\ \langle \mathcal{DN}_{01}^d, \nu_d^1 \rangle \psi_1^d + \langle \mathcal{DN}_{02}^d, \nu_d^2 \rangle \psi_2^d + \mathcal{DN}_{00}^d \psi_0^d &= \beta \psi_0^u, \\ \langle \nu_d^2 \mathcal{DN}_{21}^d \nu_d^1 \rangle \psi_1^d + \langle \nu_d^2 \mathcal{DN}_{22}^d \nu_d^2 \rangle \psi_2^d + \langle \nu_d^2 \mathcal{DN}_{20}^d \rangle \psi_0^d &= 0, \\ \langle \nu_u^1 \mathcal{DN}_{11}^d \nu_u^1 \rangle \psi_1^d + \langle \nu_u^1 \mathcal{DN}_{12}^d \nu_u^2 \rangle \psi_2^d + \langle \nu_u^1 \mathcal{DN}_{10}^d \rangle \psi_0^d &= 0.\end{aligned}\quad (11)$$

# Dispersion equation of a sandwich of quasi-2d lattice and 2d Landau-Zener effect.

Existence of a non-trivial solution of this linear system is guaranteed by an appropriate determinant condition. Denote

$$\langle \nu_{u,d}^s \mathcal{DN}_{11}^{u,d} \nu_{u,d}^s \rangle := d_{st}^{u,d},$$

$$\mathcal{DN}^{u,d}(p) =:$$

$$= \begin{pmatrix} d_{11}^{u,d} & d_{12}^{u,d} & \langle \nu^1, \mathcal{DN}_{10}^{u,d} \rangle \\ d_{21}^{u,d} & d_{22}^{u,d} & \langle \nu^2, \mathcal{DN}_{20}^{u,d} \rangle \\ \langle \mathcal{DN}_{01}^{u,d}, \nu_u^1 \rangle & \langle \mathcal{DN}_{02}^{u,d}, \nu_{u,d}^2 \rangle & \mathcal{DN}_{00}^{u,d} \end{pmatrix},$$

$$\mathcal{DN}_T^{u,d}(p) =:$$

# Dispersion equation of a sandwich of quasi-2d lattices and 2d Landau-Zener effect.

$$= \begin{pmatrix} \langle \nu_{u,d}^1 \mathcal{DN}_{11}^{u,d} \nu_{u,d}^1 \rangle & \langle \nu_{u,d}^1 \mathcal{DN}_{12}^{u,d} \nu_{u,d}^2 \rangle \\ \langle \nu_{u,d}^2 \mathcal{DN}_{21}^{u,d} \nu_{u,d}^1 \rangle & \langle \nu_{u,d}^2 \mathcal{DN}_{22}^{u,d} \nu_{u,d}^2 \rangle \end{pmatrix}. \quad (12)$$

# Dispersion equation of a sandwich of quasi-2d lattices and 2d Landau-Zener effect.

Then the determinant condition, because of  $\nu^s = \nu^s(p_s)$ , gives the dispersion equation

$$\beta^{-2} \det \mathcal{DN}^u \det \mathcal{DN}^d + \det \mathcal{DN}_T^u \det \mathcal{DN}_T^d = 0. \quad (13)$$

In particular, if  $\beta \rightarrow \infty$ , the linear system splits into a pair of independent blocks, corresponding to the upper and lower period, with the dispersion equations

$$\det \mathcal{DN}_T^u = 0 \text{ and } \det \mathcal{DN}_T^d = 0$$

similar to ones we obtained in previous section. If  $\beta$  is large, then the intersection of terms

$$\det \mathcal{DN}_T^u(p) \det \mathcal{DN}_T^d(p) = 0$$

is transformed into a quasi-intersection.

# Dispersion equation of a sandwich of quasi-2d lattices and 2d Landau-Zener effect.

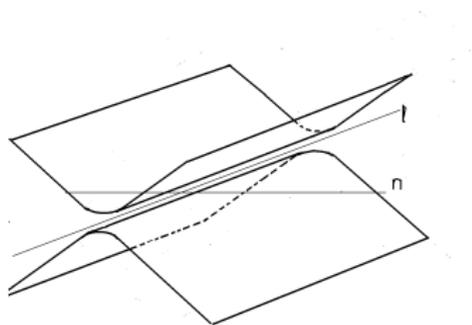


Figure: Two-dimensional Landau-Zener effect.

# Dispersion equation of a sandwich of quasi-2d lattice and 2d Landau-Zener effect.

The transport properties for large  $\beta$  near to the intersection of the unperturbed terms ( for  $\beta = \infty$ ) are defined by the tensor of second derivatives of  $\lambda$  with respect to the quasi-momentum  $p$ . In particular, the mobility of the charge carriers at the quasi-intersection is defined by the tensor  $m^{-1} = \left\{ \frac{\partial \lambda}{\partial p_s \partial p_t} \right\}_{s,t=1}^{s,t=2}$  of the second derivatives of the dispersion function  $\lambda(\vec{p})$ .

# Dispersion equation of a sandwich of quasi-2d lattices and 2d Landau-Zener effect.

For a weak interaction of the layers, the maximal eigenvalue of the tensor ( and hence the minimal effective mass and maximal mobility ) is observed on the quasi-momenta plane in the direction  $n$  orthogonal to the intersection  $l$  of the tangent planes of the dispersion surfaces of the upper and lower layers of the unperturbed sandwich. Depending on position of the Fermi level of the sandwich of lattices the charge carriers are either electrons or holes. Suggested in this paper analysis of the Bloch functions of 2d periodic lattices may serve a basement for calculation of the correlations of the wave-functions initially obtained in form of the Slater determinants, see the corresponding remark in [7] p. 293.

# Conclusion

The physical approach and the mathematical technique suggested above for analysis of the resonance processes on the periodic systems of quantum dots are based on fitted “zero-range” solvable models, which has mathematical roots in the von Neumann operator extension theory, see [14]. Though the discovery of the theory was done by John von Neumann based on a deep physical motivation, physicists never used it, in original von Neumann form, before 1964, when the seminal paper [8] was published, where the direct connection between E. Fermi zero-range potential see [12] and von Neumann theory was established.

# Conclusion

Yet another 50 years were needed to notice that the zero-range model can be fitted, based on a special choice of the inner structure and another another 20 years were needed to see, that the fitted zero-range model may be used as a first approximation - “jump-start”- in the modified analytic perturbation procedure. Now we see some prospects of using of this mathematical technique for analysis of experimental results obtained in the studies of the edge channels in the ultra-narrow quantum wells as well as high mobility of charge carriers in self-assembled Silicon-based low-dimensional periodic structures.

# Conclusion

Specifically, this theoretical analysis allows to observe the influence of the quantum dots and single impurity centers embedded in the edge channels on the characteristics of the spin-dependent scattering, revealed by the quantum Hall effect and quantum spin Hall effect measurements as well as features revealed by the electrically-detected electron paramagnetic resonance, see [1, 5, 6]. We hope that the new analytic constructions discussed above based on von Neumann operator extension theory, will find wide a range of applications in solid-state physics.

# Acknowledgement

The authors are grateful to Kyle Beloy and Anastasia Borschevsky for an important remark concerning the leading role of 2-electrons correlations in coupled clusters techniques and R. Bartlett for encouraging discussion of basic ideas and state of art of the coupled-clusters theory, as well as the reprint [7] provided.

-  1. N.T. Bagraev, A.D. Bouravleuv, L.E. Klyachkin, A.M. Malyarenko, I.A. Shelykh. *Negative-U properties for a quantum dot: Proc. of the 22nd International Conference on Defects in Semiconductors (ICDS-22)*, Aarhus, Denmark, Physica B, v.340-342, p.p.1061-1064, 2003.
-  2. N. Bagraev, A. Buravlev, L. Klyachkin, A. Malyarenko, W. Gehlhoff, Yu. Romanov, S. Rykov. *Local tunnel spectroscopy of silicon structures* Physics and techniques of semiconductors, (Russian), **39**, 6, (2005) pp 716-727.
-  3. N. Bagraev, W. Gehlhoff, L. Klyachkin, A. Malyarenko and V. Romanov *Superconductivity in Silicon Nanostructures* In : Physica C, Superconductivity, Volumes 437-438, 15 May 2006, pages 21-24, Proceedings of the IV-th International Conference on Vortex matter in

Nanostructures Semiconductors, Vortex IV, DOI  
10.1016/j.physc.2005.12.011.



4. N.Bagraev, A.Mikhailova, B. Pavlov, L.Prokhorov, A.Yafyasov *Parameter regime of a resonance quantum switch*, Phys. Rev. B, 71, 165308 (2005), pp 1-16.



4. N.T. Bagraev, N.G. Galkin, W. Gehlhoff, L.E. Klyachkin, A.M. Malyarenko: *Phase and amplitude response of the 0.7 feature caused by holes in silicon one-dimensional wires and rings*. J. Phys.:Condens. Matter, v.20, p.p.164202-12, 2008.



5. N.T. Bagraev, W. Gehlhoff, L.E. Klyachkin, A.A. Kudryavtsev, A.M. Malyarenko, G.A. Oganesyanyan, D.S. Poloskin, V.V. Romanov *Spin-dependent transport of holes in silicon quantum wells confined by superconductor barriers* Physica C, v.468, p.p.840-843, 2008.

-  6. R.J. Bartlett, M. Musial *Coupled -cluster theory in quantum chemistry*, Reviews of Modern Physics, **79**, 1, Jan. 2007, 291-351.
-  F.A.Berezin, L.D.Faddeev *A remark on Schrödinger equation with a singular potential* Dokl. AN SSSR, **137** (1961) pp 1011-1014.
-  7. J. Brüning, G. Martin, B. Pavlov *Calculation of the Kirchhoff coefficients for the Helmholtz resonator*, Russ. J. Math. Phys., **16**, (2009), no. 2, 188–207.
-  8. J. Callaway *Energy band theory*, Academic Press, NY-London, 1964

-  9. Y.N. Demkov, P.B.Kurasov, V.N. Ostrovski  
*Double-periodical in time and energy solvable system with two interacting set of states*, Journal of Physics A, Math. and General, **28**, (1995), p.434.
-  E.Fermi *Sul motto dei neutroni nelle sostanze idrogenate* (in Italian) Richerka Scientifica **7** p 13 (1936)
-  10. C. Fox, V. Oleinik, B. Pavlov *A Dirichlet-to-Neumann approach to resonance gaps and bands of periodic networks*) Contemporary mathematics, **412**, (2006)  
Proceedings of the Conference: Operator Theory and mathematical Physics, Birmingham, Alabama, 2005, 151-169.

-  11. J. von Neumann *Mathematical foundations of quantum mechanics* Twelfth printing. Princeton Landmarks in Mathematics. Princeton Paperbacks. Princeton University Press, Princeton, NJ, (1996)
-  12. K.Novoselov, A. Geim, S.Morozov, D. Jiang, I. Katsnelson, I. Grigorieva, S. Dubonos *Two-dimensional gas of massless Dirac fermions in graphen*, Nature, **438**, (2005), 197-200.
-  13. J. Paldus, J. Cizek *Correlation Problem in Atomic and Molecular Systems IV. Extended coupled pair Many-Electron Theory and its Application to the BH<sub>3</sub> Molecule* In: Physical Reviews A, **8**, 1, (1972) pp 50-67.

# Bibliography VI

-  14. B. Pavlov *S-Matrix and Dirichlet-to-Neumann Operators*  
In: Encyclopedia of Scattering, ed. R. Pike, P. Sabatier,  
Academic Press, Harcourt Science and Tech. Company  
(2001) 1678-1688
-  15. J. Sylvester, G. Uhlmann *The Dirichlet to Neumann map  
and applications*. Proceedings of the Conference “ Inverse  
problems in partial differential equations”, Arcata,1989,  
SIAM, Philadelphia, 101 (1990)
-  16. C. Zener *Non-adiabatic crossing of energy -levels* ,  
Proc. Royal Soc. A, **137**,(1932) p.696.
-  17. J.Ziman, N.Mott,P.Hirsch *The Physics of Metals*  
London, Cambridge, 1969.
-  18. J. Ziman *Electrons and phonons: the theory of transport  
phenomena in solids* Oxford University Press 1960