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Landau-Zener effect on quasi-2D periodic sandwich

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Abstract

The Bloch-waves in 1D periodic lattices are constructed based on transfer-matrix approach, with a complete system of solutions of the Cauchy problem on the period. This approach fails for the multi-dimensional Schrödinger equations on periodic lattices, because the Cauchy problem is ill-posed the elliptic partial equations. In our previous paper [8] we suggested another procedure for calculation of the Bloch functions of 2D Schrödinger equation based on Dirichlet-to-Neumann map, to substitute the transfer -matrix approach. In this paper we suggest a computer realization of the procedure.

Outline

1. Transfer- matrix and DN-map approach to Bloch-functions of 1D periodic lattices.
2. DN-map approach to Bloch-functions on a quasi-2D periodic lattice.
3. Finite-dimensional low-energy approximation for the dispersion of a 2D periodic lattice
4. Landau-Zener phenomenon for quazi-2D periodic sandwich.
5. Dispersion equation for a sandwich with a resonance barrier.
6. Landau-Zener enhancement of the BCS gap and a possibility of the HTSC on a quasi-2D periodic sandwich .

Transfer- matrix and DN-map approach for 1D periodic lattices

Study of basic quantum features of solids is reduced to one-body spectral problem on periodic lattices and construction of the quasi-periodic solutions of the one-body Schrödinger equation - Bloch-functions, see [16, 18]. In 1D case the 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 $\theta(0) = 1, \theta'(0) = 0,\ \varphi(0) = 0, \varphi'(0) = 1$:

$$-\theta'' + q\theta = \lambda\theta,\ -\varphi'' + q\varphi = \lambda\varphi,\ \text{and} \qquad (1)$$

Transfer- matrix and DN-map approach for 1D periodic lattices

Bloch function is a linear combination $\chi = \theta + \mu\varphi$ which satisfies the quasi-periodic boundary conditions

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

On the spectral bands σ_s $\mu = e^{ipa}$ with a real quasi-momentum p. The spectral bands are defined by the condition $-1 \leq \mathcal{T}(\lambda) \leq 1$ imposed on the trace $\mathrm{Tr}\,\mathcal{T}(\lambda) = \frac{1}{2}[\theta(a) + \varphi'(a)]$ of the transfer matrix

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

Transfer- matrix and DN-map approach for 1D periodic lattices

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

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

This means that the Cauchy data $(1, m)$ of the Bloch function give an eigenvector of the transfer matrix, and μ is the corresponding eigenvalue:

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

which is equivalent to the equation $\mu^2 - [\theta(a) + \varphi'(a)]\,\mu + 1 = 0$. Hence the dispersion $\lambda = \lambda(p)$ and the position of the spectral bands $\sigma : |\mu| = 1$ is defined by the trace of the transfer matrix, see Fig.1.

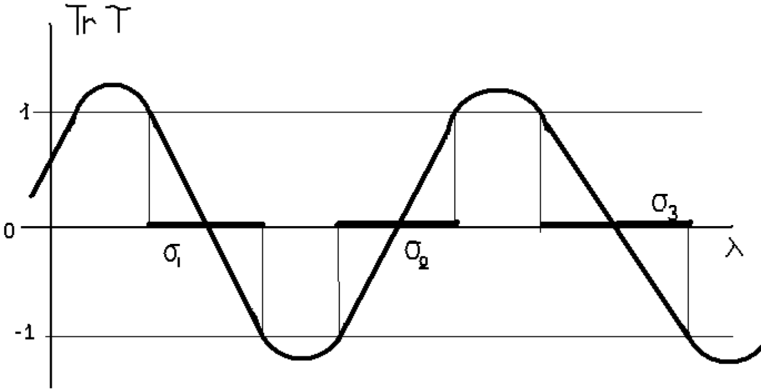


Figure: 1. The spectral bands σ_s of the 1D periodic problem found from the condition $-1 \leq Tr\ \mathcal{T} < 1$.

Transfer- matrix and DN-map approach for 1D periodic lattices

The above "transfer-matrix path" to construction of Bloch functions fails in the case of multi-dimensional periodic lattices, because the Cauchy problem is ill-posed for partial elliptic equations. Fortunately this is not an only way even in 1D case. One can also obtain the Bloch solution from analysis of some boundary problem. Indeed, consider,- instead of the standard solutions θ, φ of the Cauchy problem,- others standard 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. 2 below, (1), (2).

Transfer- matrix and DN-map approach for 1D periodic lattices

The 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.

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

Transfer- matrix and DN-map approach for 1D periodic lattices

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

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

such that

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

Then the quasi-momentum exponential $e^{ipa} = \mu$ can be found from the quadratic equation

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

which can be re-written as

Transfer- matrix and DN-map approach for 1D periodic lattices

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

Here the coefficient in front of μ is equal again to
Tr $\mathcal{T} = \mu + \mu^{-1}$.

Transfer- matrix and DN-map approach for 1D periodic lattices

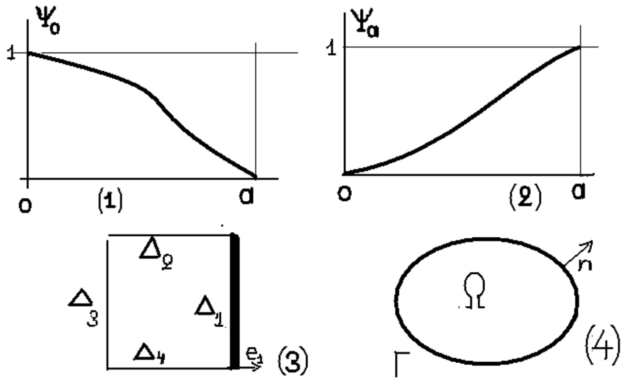


Figure: 2. Standard solutions ψ_0 (1) and ψ_a (2) of the 1D boundary problem. Standard solutions ψ_{Δ^1}, ψ_{Δ^2} of the 2D boundary problem on the square period (3). Standard solutions of the boundary problems on the domain with a smooth boundary (4).

Transfer- matrix and DN-map approach for 1D periodic lattices

Then the Bloch solution can be constructed of the standard solutions ψ_0, ψ_a as $\chi(x) = \chi(0)\left[\psi_0(x) + e^{ipa}\psi_a(x)\right]$, with selected constant $\chi(0)$. This naive approach to construction of the Bloch function, contrary to the former one (based of the transfer matrix) can be extended to multidimensional lattices, because it is dealing with objects naturally defined in multidimensional environment. Indeed, one can define, based on ψ_0, ψ_a the Dirichlet-to-Neumann map on the period, transferring the Dirichlet data $u(0), u(a)$ of the solution on the boundary into the Neumann data $u'(0), u'(a)$.

Transfer- matrix and DN-map approach for 1D periodic lattices

$$\begin{pmatrix} \psi_0'(0) & \psi_a'(0) \\ \psi_0'(a) & \psi_a'(a) \end{pmatrix} \begin{pmatrix} u(0) \\ u(a) \end{pmatrix} = \begin{pmatrix} u'(0) \\ u'(a) \end{pmatrix} \equiv \mathcal{DN} \begin{pmatrix} u(0) \\ u(a) \end{pmatrix}. \tag{3}$$

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 homogeneous equation with respect to the the independent variables $(u(0), u'(0))$:

$$\begin{pmatrix} \psi_0'(0) & \psi_a'(0) \\ \psi_0'(a) & \psi_a'(a) \end{pmatrix} \begin{pmatrix} 1 \\ \mu \end{pmatrix} \chi(0) = \begin{pmatrix} 1 \\ \mu \end{pmatrix} \chi'(0) \qquad (4)$$

Transfer- matrix and DN-map approach for 1D periodic lattices

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 (2). The basic feature of the this approach based on boundary problem is the Dirichlet-to-Neumann map, introduced in (3). The cauchy problem is present just in form of the variables $(u(0), u'(0))$, which can be considered as independent due to uniquness theorem : $(u(0) = 0, u'(0) = 0$ involves vanishing of the corresponding solution of the Schrödinger equation $-u'' + qu - \lambda u = 0)$.

The proposed way to construction of Bloch functions does not use existence of solution 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 multidimensional case, though existence of solution of Cauchy problem is absent. Fortunately we do not need existence on this way. An only,- yet non-essential- difference of the general multidimensional path from the one-dimensional version of it 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.

DN-map approach to Bloch-functions on a quasi-2D periodic lattice.

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

$$- \triangle \psi_s + q\psi_s = \lambda\psi_s, \ \psi_s\Big|_\Gamma = \psi_s^\Gamma$$

Due to uniqueness theorem for 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. In particular:

DN-map approach to Bloch-functions on a quasi-2D periodic lattice.

This fact allows 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 normal derivative

$$\mathcal{DN} : u_\Gamma \longrightarrow \frac{\partial u}{\partial n}\Big|_\Gamma, \tag{5}$$

see [22] for 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 $\int_\Gamma \bar{u}_l \, \frac{\partial u_m}{\partial n} d\Gamma \equiv \langle u_l, \mathcal{DN} u_l \rangle$.

DN-map approach to Bloch-functions on a quasi-2D periodic lattice.

The Green formula allows to transform the matrix element into the bilinear form of the Schrödinger operator.

$$\langle u_l, \mathcal{DN} u_m \rangle = \int_\Omega [\nabla \bar{u}_l \nabla u_m + q \bar{u}_l\, u_m - \lambda \bar{u}_l\, u_m]\, d\Omega. \qquad (6)$$

This formula permits 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. In the case when λ is close to a Dirichlet eigenvalue, it is more convenient to calculate the matrix elements of the Neumann-to-Dirichlet map. It is done based on the same formula (), but beginning from solution of a sequence of Neumann problems for a smooth orthogonal basis $\{\rho_s\}$ in $L_2(\Gamma)$

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

DN-map approach to Bloch-functions on a quasi-2D periodic lattice.

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

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

$$\langle \mathcal{N}\mathcal{D}\rho_l, \rho_m \rangle = \int_{\Omega} [\nabla \bar{v}_l \nabla v_m + q\bar{v}_l\, v_m - \lambda \bar{v}_l\, v_m]\, d\Omega. \qquad (7)$$

Once the Neumann-to-Dirichlet map is constructed, the Dirichlet-to-Neumann map , if exists for given λ, can be obtained as inverse it the former, $\mathcal{D}\mathcal{N}\,\mathcal{N}\mathcal{D} = I$.

DN-map approach to Bloch-functions on a quasi-2D periodic lattice.

Consider the quasi- 2D periodic lattice with a cubic period, see Fig. **??**, and the Schrödinger operator $Lu = - \triangle u + q(x)u$ on the lattice, with periodic potential $q : q(x^1 + ma, x^2 + na), m = \pm 1, \pm 2, \dots,$ zero boundary conditions on the lower and the upper lids $\Gamma_0^3 : x^3 = 0$, $\Gamma_h^3 : x^3 = h$ of the lattice. The whole spectral problem on the lattice is reduced to the spectral problem on the period, with the same boundary conditions on the lids $\Gamma_{0,h}^3$, and the quasi-periodic conditions on the vertical walls $\Gamma_{0,a}^{1,2}$. The positive normale on $\Gamma_a^{1,2}$ is defined by the orts e_1, e_2, and the positive normals on the walls $\Gamma_0^{1,2}$ are $-e_1, -e_2$.

DN-map approach to Bloch-functions on a quasi-2D periodic lattice.

The quasi-periodic boundary conditions permit to eliminate the boundary data $u\Big|_{\Gamma_0^{1,2}}, \frac{\partial u}{\partial n}\Big|_{\Gamma_0^{1,2}}$ on the walls $\Gamma_0^{1,2}$:

$$u\Big|_{\Gamma_0^{1,2}} = e^{-ip_{1,2}a} u\Big|_{\Gamma_a^{1,2}}, \ \frac{\partial u}{\partial n}\Big|_{\Gamma_0^{1,2}} = e^{-ip_{1,2}a} \frac{\partial u}{\partial n}\Big|_{\Gamma_a^{1,2}}.$$

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

DN-map approach to Bloch-functions on a quasi-2D periodic lattice.

$$\begin{pmatrix} \left.\frac{\partial u}{\partial n}\right|_{\Gamma_0^1} \\ \left.\frac{\partial u}{\partial n}\right|_{\Gamma_0^2} \\ \left.e^{-ip_{1,2}a}\frac{\partial u}{\partial n}\right|_{\Gamma_a^1} \\ \left.e^{-ip_{1,2}a}\frac{\partial u}{\partial n}\right|_{\Gamma_a^2} \end{pmatrix} \equiv \begin{pmatrix} \frac{\partial \vec{u}_a}{\partial n} \\ \mu^{-1}\frac{\partial \vec{u}_a}{\partial n} \end{pmatrix} = \mathcal{DN} \begin{pmatrix} \left.u\right|_{\Gamma_a^1} \\ \left.u\right|_{\Gamma_a^2} \\ \left.e^{-ip_1 a}u\right|_{\Gamma_a^1} \\ \left.e^{-ip_2 a}u\right|_{\Gamma_a^2} \end{pmatrix} \tag{8}$$

DN-map approach to Bloch-functions on a quasi-2D periodic lattice.

$$\mathcal{DN}\begin{pmatrix} u\Big|_{\Gamma_a^1} \\ u\Big|_{\Gamma_a^2} \\ e^{-ip_1 a}u\Big|_{\Gamma_a^1} \\ e^{-ip_2 a}u\Big|_{\Gamma_a^2} \end{pmatrix} \equiv \mathcal{DN}\begin{pmatrix} \vec{u}_a \\ \mu^{-1}\,\vec{u}_a \end{pmatrix}. \tag{9}$$

Here $\mu = [\mu_1, \mu_2] = [e^{1p_1 a}, e^{1p_2 a}]$ is a diagonal matrix.

DN-map approach to Bloch-functions on a quasi-2D periodic lattice.

The DN-map $\mathcal{DN}$ can be represented in the 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.

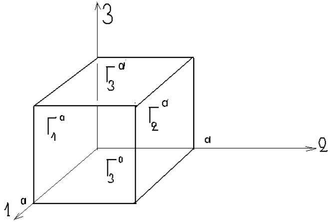


Figure: 3. 3D-period of the quasi-2D lattice, with zero boundary conditions on Γ^3_α.

DN-map approach to Bloch-functions on a quasi-2D periodic lattice.

Matrix elements of the DN map connect the Dirichlet data on Γ_{α}^{ik} with Neumann data on $\Gamma_{\alpha'}^{jl}$.

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

DN-map approach to Bloch-functions on a quasi-2D periodic lattice.

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

DN-map approach to Bloch-functions on a quasi-2D periodic lattice.

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 $\frac{\partial \vec{u}_a}{\partial n}, \frac{\partial \vec{u}_0}{\partial n}$. 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 vector-functions $\left(\vec{u}_a, \frac{\partial \vec{u}_a}{\partial n} \right)$.

DN-map approach to Bloch-functions on a quasi-2D periodic lattice.

$$\begin{pmatrix} \frac{\partial \vec{u}_a}{\partial n} \\ \mu^{-1} \frac{\partial \vec{u}_a}{\partial n} \end{pmatrix} = \begin{pmatrix} \mathcal{DN}_{aa} & \mathcal{DN}_{a0} \\ \mathcal{DN}_{0a} & \mathcal{DN}_{00} \end{pmatrix} \begin{pmatrix} \vec{u}_a \\ \mu^{-1} \vec{u}_a \end{pmatrix}. \qquad (10)$$

DN-map approach to Bloch-functions on a quasi-2D periodic lattice.

Eliminating $\frac{\partial \vec{u}_a}{\partial n}$ we conclude that a nontrivial solution of the equation 10 exists if and only if zero is an eigenvalue of the operator:

$$[\mu\mathcal{DN}_{0a}\mu + \mu\mathcal{DN}_{00} - \mathcal{DN}_{aa}\mu - \mathcal{DN}_{00}]\,\vec{u}_a = 0. \qquad (11)$$

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

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

The equation (11) is an analog of the quadratic equation (2), but question on existence of the corresponding solution of it in general case is not understood yet.

DN-map approach to Bloch-functions on a quasi-2D periodic lattice.

Fortunately the physically meaningful spectral problem on the cubic periodic lattice, see for instance the romboidal periods , see Fig. 4, with relatively narrow connecting channels Γ^i_α, $\alpha = 0, a; 1 = 1, 2$, gives a chance of simplification of the model down to the solvable level.

DN-map approach to Bloch-functions on a quasi-2D periodic lattice.

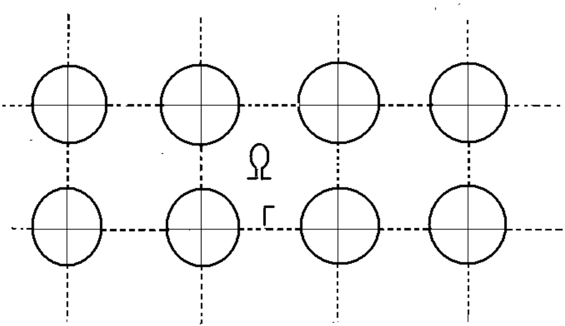


Figure: 4. 2D periodic lattice with romboidal periods

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

The structure of branches of the wave-functions connecting neighboring periods is defined mainly by the the eigenfunctions of the conductivity band and by the covalent bonds, formed by the upper orbitals on the period.
The lower orbitals are essentially localized inside the period. This observation allows to substitute the spectral problem on the whole periodic lattice by one supplied with additional "partial" zero boundary conditions on the contacts Γ^i_α of the neighboring periods applied on the orthogonal complement $N \subset L_2(\Gamma)$ of the boundary space of eigenfunctions of the valent and conductivity bands and the Dirichlet zero boundary condition on the orthogonal complement:

$$P_N u\Big|_{\Gamma^l_0} = e^{-ip_l a} P_N u\Big|_{\Gamma^l_0};\ \ P_N \frac{\partial u}{\partial n}\Big|_{\Gamma^l_0} = e^{-ip_l a} P_N \frac{\partial u}{\partial n}\Big|_{\Gamma^l_a};\ \ P_N^{\perp} u\Big|_{\Gamma^l} = 0. \tag{12}$$

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

The structure of the corresponding spaces $N, N^{\perp}$ depends on the energy, but for low temperature the energy is defined by the Fermi level Λ_F of the material, thus N can be selected independently of energy. Then the above boundary conditions (12) define, together with the potential q and the corresponding differential expression $Lu = -\triangle u + qu$ define a selfadjoint operator L_N on the period, with *partial quasi-periodic* boundary condition in $N \subset L_2(\Gamma)$. In factds of the contact space is the main parameter of our one-body model of the 2D periodic lattice. The freedom of the choice can be used with regard of extended experience of quantum chemistry in understanding of valent bonds and conductivity in solids.

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

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

$$-\triangle u + qu = \lambda u, P_N^{\perp} u\Big|_{\Gamma^l} = 0,\ P^N u\Big|_{\Gamma^l} = u_\Gamma^N \in N. \tag{13}$$

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

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

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

Then the dispersion equation of the model with selected contact space N is obtained in the same form (11) via substitution of the standard DN- map by the partial DN map

$$\left[\mu \mathcal{DN}_{0a}^{N} \mu + \mu \mathcal{DN}_{00}^{N} - \mathcal{DN}_{aa}^{N} \mu - \mathcal{DN}_{00}^{N}\right] \vec{u}_a = 0. \tag{14}$$

The ultimate equation, contrary to (11), is a finite-dimensional, which allows to obtain the dispersion equation for the model periodic quasi-2D lattice in explicit form. Indeed, assume that there exist an eigenvalue $\lambda_1^D \approx \Lambda^F$ of the relative Dirichlet problem on the period, with an eigenfunction φ_1^D, close to the Fermi level Λ^F.

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

Then, for low temperature, the relative DN-map is substituted, on the temperature interval near to the Fermi level $\Lambda^F - 2m\kappa T\hbar^{-2}, \Lambda^F + 2m\kappa T\hbar^{-2}$, by the sum of a one-dimensional polar term and a correcting term

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

and represented by a matrix according to the decomposition of $N = \sum_{i=1,2,\alpha=0,a} N(\Gamma^i_\alpha)$. Then 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 (11)

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

$$\left[\mu Q^N_{0a}\mu + \mu Q^N_{00} - Q^N_{aa}\mu - Q^N_{00}\right] \vec{u}_a +$$
$$(\lambda - \lambda^D_1)\left[\mu B^N_{0a}\mu + \mu B^N_{00} - B^N_{aa}\mu - B^N_{00}\right] \vec{u}_a = 0, \qquad (15)$$

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

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

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

$$\frac{1}{c^2}\frac{\partial^2 u^1}{\partial t^2} = \frac{\partial^2 u^1}{\partial x^2} + \varepsilon^2 u^2, \;\; \frac{1}{c^2}\frac{\partial^2 u^2}{\partial t^2} = \frac{\partial^2 u^2}{\partial x^2} + \varepsilon^2 u^1,$$

manufactured of a magnetic material, weakly interacting due to different ($\varepsilon^2 > 0$) polarity of strings. Re-writing the above linear system in terms of Fourier-dual variables τ, ξ (the frequency and the momentum) as

$$\frac{1}{c^2}\tau^2 \tilde{u}^1 = \xi^2 \tilde{u}^2 - \varepsilon^2 \tilde{u}^2, \; \frac{1}{c^2}\tau^2 \tilde{u}^2 = \xi^2 \tilde{u}^1 - \varepsilon^2 \tilde{u}^1$$

yields a dispersion equation in the form of a determinant condition for the Fourier-dual variables $p^2 = c^{-2}\tau^2 + \varepsilon^2$.

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

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 for $\varepsilon = 0$, but form two branches of a hyperbola for $\varepsilon > 0$.

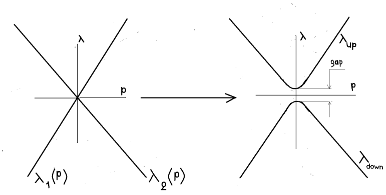


Figure: 5. One dimensional Landau-Zener effect.

Landau-Zener phenomenon for quasi-2D periodic sandwich.

The Landau-Zener effect is precisely the transformation of the crossing of the terms $\lambda_1(p), \lambda_2(p)$ for $\varepsilon = 0$, see Fig 5, into the "quasi-crossing" for $\varepsilon > 0$.This effect was first observed ,[30], on 1D periodic lattices with use of transfer-matrices , see for instance [12].

Landau-Zener phenomenon for quazi-2D periodic sandwich.

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 [27, 19, 13].

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

The recent discovery of quasi-relativistic behavior of terms in man-made bi-layer periodic quasi-two-dimensional lattices, see [5], suggests that the weak interaction of two-dimensional periodic lattices can be used as a source of various artificial structures with useful and interesting transport properties. Study of the Landau-Zener transformation in 2D case requires new analytic machinery, since the ID technique, based on the transfer-matrix, fails because of "ill-posedness" of the Cauchy problem for Schrödinger equation on a square period. We consider a periodic 2D sandwich based on Dirichlet-to-Neumann technique developed in previous section.

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

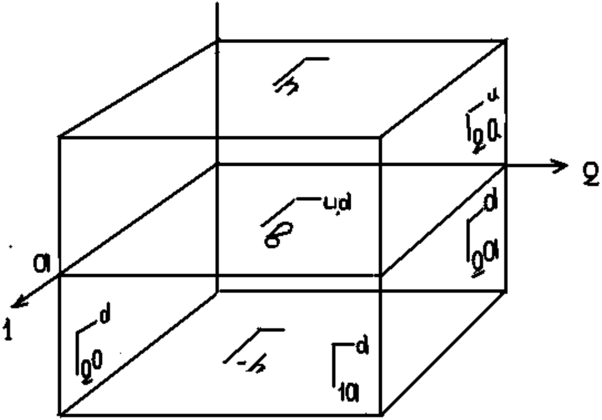


Figure: 6. Two-storey period of the periodic quasi-2D sandwich lattice.

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

Consider 2-storey period, see Fig 6 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 $\Gamma_b^{\pm}$. Denoting by $n_b^{d,u}$ the outer normals on both sides $\Gamma^{(}u, d)_b$ of the barrier, we represent the boundary condition on Γ_b as

$$P_{N_b}\left[\frac{\partial V^u}{\partial n^u}\Big|_{\Gamma_b^u} + \frac{\partial V^d}{\partial n^d}\Big|_{\Gamma_b^d}\right] + \beta V_b = 0, \quad \text{with} \quad V_b = P_{N_b} V^d\Big|_{\Gamma_b^d} = P_{N_b} V^u\Big|_{\Gamma_b^u}, \tag{16}$$

under continuity of the wave-function on the potential barrier and a jump of the normal derivative $\frac{\partial V^u}{\partial n^u}\Big|_{\Gamma_b^u} + \frac{\partial V^d}{\partial n^d}\Big|_b^d \equiv -\left[\frac{\partial V}{\partial n}\right]\Big|_{\Gamma_b}$

depending on the value of the N_b projection $P_{N_b} V^u\Big|$ of the

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

Once the magnitude of the tunneling constant β is fixed, we could consider the DN-map of the two-storey period with the joint vertical walls $\Gamma_{i,\alpha} = \Gamma^u_{i,\alpha} \cup \Gamma^d_{i,\alpha}$, and $N_i = N^u_i \cup N^d_i$ Then the dispersion equation for the 2D sandwich is obtained based in the previous formulae (14,15). More interesting is to observe the behavior of the dispersion surfaces in dependance of the the tunneling parameter β. To do that we consider the relative DN-maps of the upper and the lower storeys Ω^u, Ω^d of the whole 2-storey period Ω of the sandwich. Denote by N^u_1, N^d_i, N_b the contact subspaces associated with the corresponding walls $\Gamma^u_{\alpha,i}, \Gamma^u_{\alpha,i}, \Gamma_b$ and by $N^{u,\perp}_1, N^{d,\perp}_i, N^{\perp}_b$ the relevant orthogonal complements in the spaces of square-integrable functions on the walls.

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

$$\mathcal{DN}^u = \begin{pmatrix} \mathcal{DN}^u_{aa} & \mathcal{DN}^u_{a0} & \mathcal{DN}^u_{ab} \\ \mathcal{DN}^u_{0a} & \mathcal{DN}^u_{00} & \mathcal{DN}^u_{0b} \\ \mathcal{DN}^u_{ba} & \mathcal{DN}^u_{b0} & \mathcal{DN}^u_{bb} \end{pmatrix}, \qquad (17)$$

with 2 blocks

$$\mathcal{DN}^u_{\alpha,\alpha'} = \begin{pmatrix} P^u_1 \mathcal{DN}^u_{\alpha,\alpha'} P^u_1 & P^u_1 \mathcal{DN}^u_{\alpha,\alpha'} P^u_2 \\ P^u_2 \mathcal{DN}^u_{\alpha,\alpha'} P^u_1 & P^u_2 \mathcal{DN}^u_{\alpha,\alpha'} P^u_2 \end{pmatrix}$$

and 2×1, 1×2 and 1×1 blocks

$$\mathcal{DN}^u_{\alpha,b} = \begin{pmatrix} P^u_1 \mathcal{DN}^u_{\alpha,b} P^u_b \\ P^u_2 \mathcal{DN}^u_{\alpha,b} P^u_b \end{pmatrix}, \ \mathcal{DN}^u_{b,\alpha} = \left(P^u_b \mathcal{DN}^u_{b\alpha} P^u_1 ; P^u_b \mathcal{DN}^u_{b,\alpha} P^u_2 \right), \ \mathcal{I}$$

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

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 $\Gamma_b : P_{N_b} V\Big|_{\Gamma_b^u} = P_{N_b} V\Big|_{\Gamma_b^d}$ and the tunneling condition on the barrier

$$\left[P_{N_b} \frac{\partial V}{\partial n}\right] = \beta P_{N_b} V\Big|_{\Gamma_b}$$

is given by the block-matrix acting on the vector $\left(V_a^u, V_0^u, V_b, V_0^d, V_a^d\right)$, with 2D components

$$V_a^u \equiv (V_{a1}^u, V_{a2}^u),\; V_0^u \equiv (V_{01}^u, V_{02}^u),$$

$$V_a^d \equiv (V_{a1}^d, V_{a2}^u),\; V_0^d \equiv (V_{01}^d, V_{02}^d)$$

and 1D component V_b.

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

$$\mathcal{DN}_{2D} = \begin{pmatrix} \mathcal{DN}^u_{aa} & \mathcal{DN}^u_{a0} & \mathcal{DN}^u_{ab} & 0 & 0 \\ \mathcal{DN}^u_{0a} & \mathcal{DN}^u_{00} & \mathcal{DN}^u_{0b} & 0 & 0 \\ \mathcal{DN}^u_{ba} & \mathcal{DN}^u_{b0} & \left[\mathcal{DN}^u_{bb} + \mathcal{DN}^d_{bb}\right] & \mathcal{DN}^d_{b0} & \mathcal{DN}^u_{ba} \\ 0 & 0 & \mathcal{DN}^d_{0b} & \mathcal{DN}^d_{00} & \mathcal{DN}^d_{0a} \\ 0 & 0 & \mathcal{DN}^d_{ab} & \mathcal{DN}^d_{a0} & \mathcal{DN}^d_{aa} \end{pmatrix}. \tag{18}$$

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

Due to partial zero condition on the walls and the lids with selected entrance 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 (18) 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

Landau-Zener phenomenon for quasi-2D periodic sandwich.

$$\mathcal{DN}_{2D} \begin{pmatrix} V_a^u \\ \mu_u^{-1} V_a^u \\ V_b \\ \mu_d^{-1} V_a^d \\ V_a^d \end{pmatrix} = \begin{pmatrix} \frac{\partial V_a^u}{\partial n} \\ -\mu_u^{-1} \frac{\partial V_a^u}{\partial n} \\ \beta\, V_b \\ -\mu_d^{-1} \frac{\partial V_a^d}{\partial n} \\ \frac{\partial V_a^d}{\partial n} \end{pmatrix} \tag{19}$$

Landau-Zener phenomenon for quasi-2D periodic sandwich.

The roles of independent variables in this equation are played by the vectors $V_a^u = (V_{a1}^u, V_{a2}^u) \in N_1^u \oplus N_2^u$, $V_a^d = (V_{a1}^d, V_{a2}^d) \in N_1^d \oplus N_2^d$ and $\frac{\partial V_a^u}{\partial n} = (\frac{\partial V_{a1}^u}{\partial n}, \frac{\partial V_{a2}^u}{\partial n}) \in N_1^u \oplus N_2^u$ and $\frac{\partial V_a^d}{\partial n} = (\frac{\partial V_{a1}^d}{\partial n}, \frac{\partial V_{a2}^d}{\partial n}) \in N_1^u \oplus N_2^u$ and vector $V_b \in N_b$. The vectors $\frac{\partial V_a^u}{\partial n}, \frac{\partial V_a^d}{\partial n}$ enter only into the right side of the equation (72) and can be easily eliminated. After that the the determinant condition of existence of the remaining linear system for (V_a^u, V_a^d, V_b) gives a dispersion equation for the quasi-2D periodic sandwich. Further simplification can be obtained via substitution of $\mathcal{DN}_{2D}$ by the rational approximation near the resonance eigenvalues $\lambda_1^u, \lambda_1^d \dots$ of the partial Dirichlet problem, similar to (14, 15) in previous section.

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

For given periodic lattice consider the periods Ω, connected with neighboring ones by a minimal set of covalent bonds. Select the entrance spaces $N_\Gamma \equiv N$ 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 on 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 on the interval of the spectral parameter close to the Fermi level. Due to uniqueness theorem of the Cauchy problem for thr Schrödinger equation the difficulties in construction of the partial DN-map near the eigenvalues of the Dirichlet problem cam be avoided via construction of the corresponding ND- map and using the connection between them $\mathcal{DN}\,\mathcal{ND} = I_N$.

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

Consider a one-pole or 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. We apply a quasi-periodic boundary conditions at the boundary for the partial boundary values $P_N V$ of the wave-function V. These boundary condition are represented as a linear system for the set of independent boundary values of the wave function and the normal derivative on the boundary. The determinant condition of existence of a nontrivial solution of the system can be represented as a dispersion relation $\lambda = \lambda(p)$ with multi-dimensional quasi-momentum p on the spectral bands $p = \bar{p}$. The graphic representation of the condition gives the diagram of the dispersion relation on the valent and conductivity bands.

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

Previous plan is applied for the sandwich, with only additional detail concerning the barrier separating the upper and lower quasi 2D lattices of the sandwich. The simplest model is given by the δ - barrier, represented by the boundary condition applied on the common boundary Γ_b of the upper and lower periods Ω^u, Ω^d in the form $\frac{\partial V^u}{\partial n^u}\Big|_{\Gamma_b} + \frac{\partial V^d}{\partial n^d}\Big|_{\Gamma_b} + \beta V\Big|_{\Gamma_b} = 0, \ \beta > 0.$

The partial DN - maps of the upper and lower periods are calculated with respect to selected entrance subspaces N^u, N^d, N_b taking into account the orbitals of electrons forming the covalent bonds between neighboring periods in the upper and lower lattices and the orbitals of the electrons tunneling through the barrier. The corresponding partial DN and ND maps of the two-storey period are obtained from the partial DN and ND maps of the upper and lower periods, calculated based on bilinear forms of the wave-functions solving the sequence of

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

Once the DN and ND maps of the two-storey period are constructed, we obtain the dispersion relation for the sandwich as a determinant condition of existence of a non-trivial solution of the linear system obtained for the independent components of the boundary values of the wave-function

$V^u\big|_{\Gamma^u} \in N_u,\ V^d\Big|_{\Gamma^d} \in N^d,\ V_b \in N_b$ and the boundary currents.

Remaining components of the boundary values and the boundary currents are eliminated due to quasi-periodic boundary condition.

Slightly more realistic models of the sandwich are obtained via imposing the barrier boundary conditions not just inside the single two-storey period , but on the whole group of the neighboring periods, taking into account the quasi-periodicity. It requires consideration of more complicated, but still elementary expressions.

Dispersion equation for a sandwich witha resonance barrier.

In previous section we modeled a straight rectangular barrier with a δ function at the mutual boundary Γ_b of the upper and lower parts $\Omega^{u,d}$ of the two-storey period: $[\frac{\partial u}{\partial n}] + \beta u\Big|_{\Gamma_b} = 0$. In [7] the barrier has resonance properties defined by the subbands of 2D holes, arising in presence of an exterior electric fie3ld and narrowing, for stronger field, to the quasi-discrete levels of the size quantization, see Fig.[**?**], when the width of the potential well at the mutual boundary of the upper(low)period and the barrier of the non-doped silicon equals to the De-Broghlie wavelength in the direction orthogonal to the boundary. Positions of the levels of the size quantization are manipulated by the voltage applied to electrodes situated above and below the barrier.

Dispe3rsion equation for a sandwich witha resonance barrier.

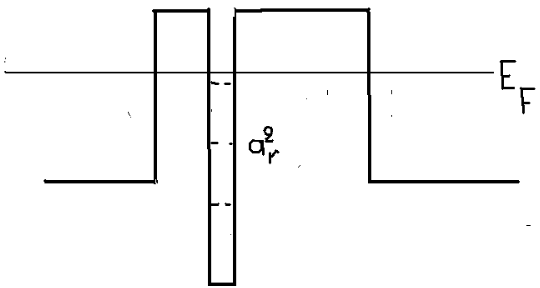


Figure: Schematic distribution of the quasi-discrete levels of the size quatization.

Dispersion equation for a sandwich with a resonance barrier.

The barrier with resonance levels can be modeled by the energy-dependent parameter β. The energy dependent parameter arises in course of construction of a zero-range model of the resonance barrier. In this section we follow [20] in defining an 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.

Dispersion equation for a sandwich with a resonance barrier.

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 N_i as a generating subspace of

$$A : \overline{\bigvee_{k>0} A^k N_{-i}} = E_A$$

such that

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

Set

$$D_0^A = (A - iI)^{-1} \left(E_A \ominus N_i \right)$$

and define the restriction of the inner Hamiltonian as

Dispersion equation for a sandwich with a resonance barrier.

Then $N_i \subset E_A$ plays the role of the deficiency subspace at the spectral point i, $\dim N_i = d,\ 2d \leq N$ and the dual deficiency subspace is $N_{-i} = \frac{A+iI}{A-iI} N_i$. The domain of the restricted operator A_0 is not dense in E_A, because A is bounded. Nevertheless, since the deficiency subspaces $N_{\pm i}$ do not overlap, the extension procedure for the orthogonal sum $l_0 \oplus A_0$ can be developed, see for instance [20]. In this case the "formal adjoint" operator for A_0 is defined on the defect $N_i + N_{-i} := \mathcal{N}$ by the von Neumann formula : $A_0^+ e \pm i\, e = 0$ for $e \in N_{\pm i}$. 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").

Dispersion equation for a sandwich with a resonance barrier.

According to the classical von Neumann construction all Lagrangian planes are parametrized by isometries $V : N_i \to N_i$ in the form

$$\mathcal{T}_V = (I - V)\, N_i.$$

It follows from [20] 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.

Note 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 [24] independently of [17]. The relevant formulas for the scattering matrix and scattered waves remain true and may be verified by the direct calculation

Dispersion equation for a sandwich with a resonance barrier.

Choose an orthonormal basis in N_i, say $\{f_s\}$, $s = 1, 2, \ldots d$, 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 N_{-i}. Under the non-overlapping condition one can use the formal adjoint operator A_0^+ defined on the defect $N_i + N_{-i} = \mathcal{N}$:

$$u = \sum_{s=1}^{d} [x_s\, f_s + \hat{x}_s\, \hat{f}_s] \in \mathcal{N}, \qquad (20)$$

by the von Neumann formula, see [1],

$$A_0^+ u = \sum_{s=1}^{d} [-i\; x_s\, f_s + i\; \hat{x}_s\, \hat{f}_s]. \qquad (21)$$

Dispersion equation for a sandwich with a resonance barrier.

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 above non-overlapping condition:

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

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

$$u = \sum_{s=1}^{d} [\xi_{+,s}\, w_{s,+} + \xi_{-,s}\, w_{s,-}]. \tag{22}$$

Dispersion equation for a sandwich with a resonance barrier.

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

$$u = \frac{A}{A - iI}\vec{\xi}_{+}^{u} - \frac{1}{A - iI}\vec{\xi}_{-}^{u}, \quad A_0^{+} u = -\frac{1}{A - iI}\vec{\xi}_{+}^{u} - \frac{A}{A - iI}\vec{\xi}_{-}^{u} \qquad (23)$$

The following formula for "integration by parts" for abstract operators was proved in [20].

lemma *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 $\vec{\xi}_{\pm}^{u}, \vec{\xi}_{\pm}^{v}$:

$$\vec{\xi}_{\pm}^{u} = \sum_{s=1}^{d} \xi_{s,\pm}^{u} f_{s,i} \in N_i, \; \vec{\xi}_{\pm}^{v} = \sum_{s=1}^{d} \xi_{s,\pm}^{v} f_s \in N_i.$$

Dispersion equation for a sandwich with a resonance barrier.

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

$$\mathcal{J}_A(u,v) = \langle A_0^+ u, v\rangle - \langle u, A_0^+ v\rangle = \langle \vec{\xi}_+^u, \vec{\xi}_-^v\rangle_N - \langle \vec{\xi}_-^u, \vec{\xi}_+^v\rangle_N. \quad (24)$$

One can see that the coordinates $\vec{\xi}_\pm^u$, $\vec{\xi}_\pm^v$ 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 will call them *symplectic coordinates* of the elements u, v. The next statement proved in [20] is the central 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.

Dispersion equation for a sandwich with a resonance barrier.

lemma *The vector-valued function of the spectral parameter*

$$u(\lambda) = \frac{A + iI}{A - \lambda I}\ \vec{\xi}^u_+ := u_0 + \frac{A}{A - iI}\vec{\xi}^u_+ - \frac{1}{A - iI}\vec{\xi}^u_-, \qquad (25)$$

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

$$\vec{\xi}^u_+ = P_{N_i}\frac{I + \lambda A}{A - \lambda I}\vec{\xi}^u_- \qquad (26)$$

Dispe3rsion equation for a sandwich witha resonance barrier.

The matrix-function

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

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 $\xi_\pm^u$ of the solution u of the adjoint equation $[A^+ - \lambda I]u = 0$ are connected via the abstract Weyl- Titchmarsh function as

$$\xi_- = \mathcal{M}\xi_+. \tag{27}$$

Dispe3rsion equation for a sandwich with a resonance barrier.

We obtain the zero-range model the resonance barrier Γ_b imposing of elements $\Psi = (\psi^d, \psi^b, \psi^u)$, $\psi^d \in L_2(\Omega^d), \psi^b \in E, \psi^u \in L_2(\Omega^u)$ boundary conditions at the barrier Γ_b. In this paper 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 [28], 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:

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

Dispe3rsion equation for a sandwich witha resonance barrier.

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

$$P_b \frac{\partial \psi^d}{\partial n\big|_{\Gamma_b^d}} + P_b \frac{\partial \psi^u}{\partial n\big|_{\Gamma_b^u}} + \bar{\beta}\xi_+ = 0, \ \ P_b \psi^d = P_b \psi^u = \beta^{-1}\xi_- \equiv \Psi_b. \tag{28}$$

Eliminating the inner components $\xi_\pm$ of the boundary values based on (27), 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:

$$\left[P_b \frac{\partial \Psi}{\partial n}\right]_b + |\beta|^2 \mathcal{M}^{-1} P_b \Psi_b - 0. \tag{29}$$

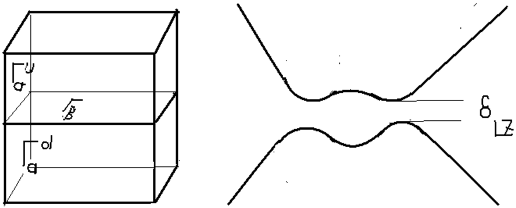
Dispe3rsion equation for a sandwich with a resonance barrier.

The dispersion equation for the sandwich with a resonance barrier is obtained from 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 the paper [7]. One can see that the of the inner Hamiltonian, which can be interpreted as the dimensional quantization levels, similarly to [28].

Landau-Zener BCS gap enhancement and a possibility of HTSC in a quasi-2D periodic sandwich.

In [7] the high-temperature superconductivity was observed in Si-B sandwich. This is interpreted as a Josephson effect due to the interaction between the Bloch functions of the upper and lower plates of the sandwich, defined by the boundary condition on the barrier Γ_b, see Fig. **??**.

Landau-Zener BCS gap enhancement and a possibility of HTSC in a quasi-2D periodic sandwich.



(1) (2)

Figure: Additional spectral Landau-0Zener gap arising from bands overlapping: (transformation of the band's crossing into the quasi-crossing).

Landau-Zener BCS gap enhancement and a possibility of HTSC in a quasi-2D periodic sandwich.

The transformation of the crossing of the corresponding 2d terms into quasi-crossings - the Landau-Zener phenomenon- is similar to one discussed in [2] for the standard and flat bands overlapping. It was shown in [2] that in one-dimensional model the spectral gap δ_{LZ}, arising due to the Landau-Zener phenomenon (Landau-Zener gap) causes the enhancement of the BKS gap, hence high-temperature stability of the superconductivity phenomenon, if the Landau-Zener phenomenon is observed at the Fermi level. In [7] additional electrodes were used to manipulate the positions of the subbands 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 sandwich structure with a resonance barrier.

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